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NUMERICAL METHODS

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JEMA41: NUMERICAL METHODS

SYLLABUS

Unit I

Finite Differences: Difference Operators–Other Difference Operators – Error propagation in a difference table.

Chapter 1: Sections -1.1 to 1.5

Unit II

Interpolation: Newton's Interpolation Formulae – Central Difference Interpolation Formulae: Gauss Forward and Backward and Sterling's (only) – Lagrange's Interpolation Formula – Divided Differences– Newton's Divided Differences formula.

Chapter 2: Sections-2.1 to 2.5

Unit III

Numerical Differentiation and Integration: Derivatives using Newton's forward difference formula–Derivatives using Newton's backward difference formula – Derivatives using central difference formula – Maxima and Minima of the Interpolating polynomial–Numerical Integration.

Chapter 3: Sections - 3.1 to 3.4

Unit IV

Numerical Solutions of Ordinary Differential Equations: Taylor's Series Method – Picard's method – Euler's method – Runge - Kutta method.

Chapter 4: Sections - 4.1 to 4.5

Unit V

Numerical Solutions of Ordinary Differential Equations: Predictor Corrector method – Milne's Method – Adams-Bash forth method.

Chapter 5: Sections 5.1 to 5.3

Text Books

S. S. Sastry, Introductory Methods of Numerical Analysis, Fifth Edition, PHI Learning Private Limited, New Delhi-1, 2009.

JEMA41: NUMERICAL METHODS

CONTENTS

Unit I

Finite Differences: Difference Operators–Other Difference Operators – Error propagation in a difference table.

Chapter 1: Sections -1.1 to 1.5

1.1 Introduction:

The statement $y = f(x), x_0 \leq x \leq x_n$ means: corresponding to every value of x in the range $x_0 \leq x \leq x_n$, there exists one or more values of y. Assuming that $f(x)$ is single-valued and continuous and that it is known explicitly, then the values of $f(x)$ corresponding to certain given values of x, say $x_0, x_1, \dots, x_n$ can easily be computed and tabulated. The central problem of numerical analysis is the converse one: Given the set of tabular values $(x_0, y_0), (x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ satisfying the relation $y = f(x)$ where the explicit nature of $f(x)$ is not known, it is required to find a simpler function, say $\phi(x)$, such that $f(x)$ and $\phi(x)$ agree at the set of tabulated points. Such a process is called interpolation. If $\phi(x)$ is a polynomial, then the process is called polynomial interpolation and $\phi(x)$ is called the interpolating polynomial. Similarly, different types of interpolation arise depending on whether $\phi(x)$ is a finite trigonometric series, series of Bessel functions, etc. In this chapter, we shall be concerned with polynomial interpolation only. As a justification for the approximation of an unknown function by means of a polynomial, we state here, without proof, a famous theorem due to Weierstrass (1885): if $f(x)$ is continuous in $x_0 \leq x \leq x_n$, then given any $\varepsilon > 0$, there exists a polynomial $P(x)$ such that

$|f(x) - P(x)| < \varepsilon,$ for all x in (x_0, x_n)

This means that it is possible to find a polynomial $P(x)$ whose graph remains within the region bounded by $y = f(x) - \varepsilon$ and $y = f(x) + \varepsilon$ for all x between x_0 and x_n, however small ε may be.

When approximating a given function $f(x)$ by means of polynomial $\phi(x)$, one may be tempted to ask: (i) How should the closeness of the approximation be measured? and (ii) What is the criterion to decide the best polynomial approximation to the function? Answers to these questions, important though they are for the practical problem of interpolation, are outside the scope of this book and will not be attempted here. We will, however, derive in the next section a formula for finding the error associated with the approximation of a tabulated function by means of a polynomial.

1.2 Errors in Polynomial Interpolation:

Let the function $y(x)$, defined by the $(n+1)$ points $(x_i, y_i), i = 0,1,2, \dots, n$, be continuous and differentiable $(n+1)$ times, and let $y(x)$ be approximated by a polynomial $\phi_n(x)$ of degree not exceeding n such that $\phi_n(x_i) = y_i, i = 0,1,2, \dots, n$ ....(1)

If we now use $\phi_n(x)$ to obtain approximate values of $y(x)$ at some points other than those defined by Equation (1), what would be the accuracy of this approximation? Since the expression $y(x) - \phi_n(x)$ vanishes for $x = x_0, x_1, \dots, x_n$, we put

$y(x) - \phi_n(x) = L\Pi_{n+1}(x)$ .... (2)

Where $\Pi_{n+1}(x) = (x - x_0)(x - x_1) \dots (x - x_n)$ ....(3)

and L is to be determined such that Equation (2) holds for any intermediate value of x, say $x = x', x_0 < x' < x_n$. Clearly,

$L = \frac{y(x') - \phi_n(x')}{\Pi_{n+1}(x')}$ ....(4)

We construct a function $F(x)$ such that $F(x) = y(x) - \phi_n(x) - L\Pi_{n+1}(x)$ ....(5)

where L is given by Equation (4) above,

It is clear that

$F(x_0) = F(x_1) = \cdots = F(x_n) = F(x') = 0$

that is, $F(x)$ vanishes $(n+2)$ times in the interval $x_0 \le x \le x_n$; consequently, by the repeated application of Rolle's theorem, $F'(x)$ must vanish $(n+1)$ times, $F''(x)$ must vanish n times, etc., in the interval $x_0 \le x \le x_n$. In particular, $F^{(n+1)}(x)$ must vanish once in the interval.

Let this point be given by $x = \xi, x_0 < \xi < x_n$. On differentiating Eq. (3.5) $(n+1)$ times with respect to x and putting $x = \xi$, we obtain

$0 = y^{(n+1)}(\xi) - L(n+1)!$

so that $L = \frac{y^{(n+1)}(\xi)}{(n+1)!}$ ....(6)

Comparison of Equations. (4) and (6) yields the results

$$y(x') - \phi_n(x') = \frac{y^{(n+1)}(\xi)}{(n+1)!}\Pi_{n+1}(x')$$

Dropping the prime on x', we obtain

$$y(x) - \phi_n(x) = \frac{\Pi_{n+1}(x)}{(n+1)!} y^{(n+1)}(\xi), x_0 < \xi < x_n \quad ....(7)$$

which is the required expression for the error. Since $y(x)$ is, generally, unknown and hence we do not have any information concerning $y^{(n+1)}(x)$, formula (7) is almost useless in practical computations. On the other hand, it is extremely useful in theoretical work in different branches of numerical analysis. In particular, we will use it to determine errors in Newton's interpolating formulae which will be discussed in Section 1.6.

1.3 Finite Differences:

Assume that we have a table of values $(x_i, y_i), i = 0,1,2, \dots, n$ of any function $y = f(x)$, the values of x being equally spaced, i.e., $x_i = x_0 + ih$, $i = 0,1,2, \dots, n$. Suppose that we are required to recover the values of $f(x)$ for some intermediate values of x, or to obtain the derivative of $f(x)$ for some x in the range $x_0 \le x \le x_n$. The methods for the solution to these problems are based on the concept of the 'differences' of a function which we now proceed to define.

1.3.1 Forward Differences:

If $y_0, y_1, y_2, \dots, y_n$ denote a set of values of y, then $y_1 - y_0, y_2 - y_1$, ..., $y_n - y_{n-1}$ are called the differences of y. Denoting these differences by $\Delta y_0, \Delta y_1, \dots, \Delta y_{n-1}$ respectively, we have

$$\Delta y_0 = y_1 - y_0, \Delta y_1 = y_2 - y_1, \dots, \Delta y_{n-1} = y_n - y_{n-1}$$

where Δ is called the forward difference operator and $\Delta y_0, \Delta y_1$, ..., are called first forward differences. The differences of the first forward differences are called second forward differences and are denoted by $\Delta^2 y_0, \Delta^2 y_1$, ... Similarly, one can define third forward differences, fourth forward differences, etc.

Thus,

$$\begin{aligned}
\Delta^2 y_0 = \Delta y_1 - \Delta y_0 &= y_2 - y_1 - (y_1 - y_0) \\
&= y_2 - 2y_1 + y_0 \\
\Delta^3 y_0 = \Delta^2 y_1 - \Delta^2 y_0 &= y_3 - 2y_2 + y_1 - (y_2 - 2y_1 + y_0) \\
&= y_3 - 3y_2 + 3y_1 - y_0 \\
\Delta^4 y_0 = \Delta^3 y_1 - \Delta^3 y_0 &= y_4 - 3y_3 + 3y_2 - y_1 - (y_3 - 3y_2 + 3y_1 - y_0) \\
&= y_4 - 4y_3 + 6y_2 - 4y_1 + y_0
\end{aligned}$$

It is, therefore, clear that any higher-order difference can easily be expressed in terms of the ordinates, since the coefficients occurring on the right side are the binomial coefficients.

Table 1.1 shows how the forward differences of all orders can be formed:

Table 1.1 Forward Difference Table

x	y_0	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
x_0	y_0	Δy_0					
x_1	y_1	Δy_1	$\Delta^2 y_0$				
x_2	y_2	Δy_1	$\Delta^2 y_1$	$\Delta^3 y_0$	$\Delta^4 y_0$		
x_3	y_3	Δy_2	$\Delta^2 y_2$	$\Delta^3 y_1$	$\Delta^4 y_1$	$\Delta^5 y_0$	$\Delta^6 y_0$
x_4	y_4	Δy_3	$\Delta^2 y_3$	$\Delta^3 y_2$	$\Delta^4 y_2$	$\Delta^5 y_1$	
x_5	y_5	Δy_4	$\Delta^2 y_4$	$\Delta^3 y_3$			
x_6	y_6	Δy_5					

In practical computations, the forward difference table can be formed in the following way. For the data points $(x_i, y_i), i = 0,1,2, \ldots, n$ and $x_i = x_0 + ih$, we have

$$\Delta y_j = y_{j+1} - y_i, j = 0,1, \ldots, n-1$$

Denoting y_j as $\mathrm{DEL}(0, j)$, the above equation can be written as

$$\Delta y_j = \mathrm{DEL}(0, j+1) - \mathrm{DEL}(0, j) = \mathrm{DEL}(1, j)$$

It follows that

$$\Delta^i y_j = \mathrm{DEL}(i-1, j+1) - \mathrm{DEL}(i-1, j)$$

which is the i th forward difference of y_j.

For the data points $(x_i, y_i), i = 0,1,2, \ldots, 6$, we have difference Table 1.2.

Table 1.2 Forward Difference Table

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
x_0	DEL(0,0)	DEL(1,0)					
x_1	DEL(0,1)	DEL(1,1)	DEL(2,0)				
x_2	DEL(0,2)	DEL(3,0)					
x_3	DEL(0,3)	DEL(1,2)	DEL(2,1)	DEL(2,2)	DEL(3,1)	DEL(4,0)	DEL(5,0)

x_4	DEL(0,4)	DEL(1,3)	DEL, 1)	DEL(3,2)	DEL(6)	DEL(5,1)	DEL(1,0)
x_5	DEL(0,5)	DEL, 4)	DEL(2,4)	DEL(3,3)			
x_6	DEL(0,6)	DEL(1,5)					

In Table 1.2

$$\begin{aligned}
\mathrm{DEL}(4,0) &= \mathrm{DEL}(3,1) - \mathrm{DEL}(3,0) \\
&= \mathrm{DEL}(2,2) - \mathrm{DEL}(2,1) - [\mathrm{DEL}(2,1) - \mathrm{DEL}(2,0)] \\
&= \mathrm{DEL}(1,3) - \mathrm{DEL}(1,2) - 2[\mathrm{DEL}(1,2) - \mathrm{DEL}(1,1)] \\
&\quad + \mathrm{DEL}(1,1) - \mathrm{DEL}(1,0) \\
&= \mathrm{DEL}(0,4) - \mathrm{DEL}(0,3) - 3[\mathrm{DEL}(0,3) - \mathrm{DEL}(0,2)] \\
&\quad + 3[\mathrm{DEL}(0,2) - \mathrm{DEL}(0,1)] - [\mathrm{DEL}(0,1) - \mathrm{DEL}(0,0)] \\
&= \mathrm{DEL}(0,4) - 4\mathrm{DEL}(0,3) + 6\mathrm{DEL}(0,2) - 4\mathrm{DEL}(0,1) + \mathrm{DEL}(0,0) \\
&= y_4 - 4y_3 + 6y_2 - 4y_1 + y_0
\end{aligned}$$

The forward difference table can now be formed by the simple statements:

```
Do i = 1(1)n
Do j = O(1)n - i
DEL(i, j) = DEL(i - 1, j + 1) - DEL(i - 1, j)
Next j
Next i
End
```

1.3.2 Backward Differences:

The differences $y_1 - y_0, y_2 - y_1, \dots, y_n - y_{n-1}$ are called first backward differences if they are denoted by $\nabla y_1, \nabla y_2, \dots, \nabla y_n$ respectively, so that

$$\nabla y_1 = y_1 - y_0, \nabla y_2 = y_2 - y_1,$$
$$\vdots$$
$$\vdots$$
$$\vdots$$
$$\nabla y_n = y_n - y_{n-1}$$

where ∇ is called the backward difference operator. In a similar way, one can define backward differences of higher orders.

Thus, we obtain

$$\nabla^2 y_2 = \nabla y_2 - \nabla y_1$$
$$= y_2 - y_1 - (y_1 - y_0) = y_2 - 2y_1 + y_0$$
$$\nabla^3 y_3 = \nabla^2 y_3 - \nabla^2 y_2$$
$$= y_3 - 3y_2 + 3y_1 - y_0, \text{ etc.}$$

With the same values of x and y as in Table 3.1, a backward difference Table 3.3 can be formed:

Table 1.3 Backward Difference Table

x	y	∇	∇^2	∇^3	∇^4	∇^5	∇^6
x_0	y_0						
x_1	y_1	∇y_1					
x_2	y_2	∇y_2	$\nabla^2 y_2$				
x_3	y_3	∇y_3	$\nabla^2 y_3$	$\nabla^3 y_3$			
x_4	y_4	∇y_4	$\nabla^2 y_4$	$\nabla^3 y_4$	$\nabla^4 y_4$		
x_5	y_5	∇y_5	$\nabla^2 y_5$	$\nabla^3 y_5$	$\nabla^4 y_5$	$\nabla^5 y_5$	
x_6	y_6	∇y_6	$\nabla^2 y_6$	$\nabla^3 y_6$	$\nabla^4 y_6$	$\nabla^5 y_6$	$\nabla^6 y_6$

1.3.3 Central Differences:

The central difference operator δ is defined by the relations

$$y_1 - y_0 = \delta y_{1/2}, y_2 - y_1 = \delta y_{3/2}, \dots, y_n - y_{n-1} = \delta y_{n-1/2}$$

Similarly, higher-order central differences can be defined. With the values of x and y as in the preceding two tables, a central difference Table 3.4 can be formed:

Table 1.4 Central Difference Table

x	y	δ	δ^2	δ^3	δ^4	δ^5	δ^6
x_0	y_0	$\delta y_{1/2}$					
x_1	y_1	$\delta y_{3/2}$	$\delta^2 y_1$	$\delta^3 y_{3/2}$			
x_2	y_2	$\delta y_{5/2}$	$\delta^2 y_2$	$\delta^3 y_{5/2}$	$\delta^4 y_2$	δ^5	
x_3	y_3	$\delta y_{7/2}$	$\delta^2 y_3$	$\delta^3 y_{7/2}$	$\delta^4 y_3$	$\delta^5 y_{7/2}$	$\delta^6 y_3$

x_4	y_4	$\delta y_{9/2}$	$\delta^2 y_4$	$\delta^3 y_{9/2}$	$\delta^4 y_4$
x_5	y_5	$\delta y_{11/2}$	$\delta^2 y_5$		
x_6	y_6				

It is clear from all the four tables that in a definite numerical case, the same numbers occur in the same positions whether we use forward, backward or central differences. Thus, we obtain

$$\Delta y_0 = \nabla y_1 = \delta y_{1/2}, \Delta^3 y_2 = \nabla^3 y_5 = \delta^3 y_{7/2}, \ldots$$

1.3.4 Symbolic Relations and Separation of Symbols:

Difference formulae can easily be established by symbolic methods, using the shift operator E and the averaging or the mean operator μ, in addition to the operators, Δ, ∇ and δ already defined.

The averaging operator μ is defined by the equation:

$$\mu y_r = \frac{1}{2}\left(y_{r+1/2} + y_{r-1/2}\right)$$

The shift operator E is defined by the equation:

$$E y_r = y_{r+1}$$

which shows that the effect of E is to shift the functional value y_r to the next higher value y_{r+1}. A second equation with E gives

$$E^2 y_r = E(E y_r) = E y_{r+1} = y_{r+2}$$

and in general,

$$E^n y_r = y_{r+n}$$

It is now easy to derive a relationship between Δ and E, for we have

$$\Delta y_0 = y_1 - y_0 = E y_0 - y_0 = (E-1) y_0$$

and hence

$$\Delta \equiv E - 1 \text{ or } E \equiv 1 + \Delta \quad \ldots\ldots\ldots.(1)$$

We can now express any higher-order forward difference in terms of the given function values. For example,

$$\Delta^3 y_0 = (E-1)^3 y_0 = (E^3 - 3E^2 + 3E - 1) y_0 = y_3 - 3y_2 + 3y_1 - y_0$$

From the definitions, the following relations can easily be established:

$\nabla = 1 - E^{-1}$

$\delta = E^{\frac{1}{2}} - E^{-\frac{1}{2}}, \quad \mu = \frac{1}{2}\left(E^{1/2} + E^{-1/2}\right),$ ……….(2)

$\Delta = \nabla E = \delta E^{1/2}.$

$\mu^2 \equiv 1 + (1/4)\delta^2$

As an example, we prove the relation

$$\mu^2 \equiv 1 + (1/4)\delta^2$$

We have, by definition,

$$\mu y_r = \frac{1}{2}\left(y_{r+1/2} + y_{r-1/2}\right)$$
$$= \frac{1}{2}\left(E^{1/2}y_r + E^{-1/2}y_r\right)$$
$$= \frac{1}{2}\left(E^{1/2} + E^{-1/2}\right)y_r.$$

Hence

$$\mu = \frac{1}{2}\left(E^{1/2} + E^{-1/2}\right)$$

and

$$\mu^2 = \frac{1}{4}\left(E^{1/2} + E^{-1/2}\right)^2$$
$$= \frac{1}{4}\left(E + E^{-1} + 2\right)$$
$$= \frac{1}{4}\left[\left(E^{1/2} - E^{-1/2}\right)^2 + 4\right]$$
$$= \frac{1}{4}\left(\delta^2 + 4\right).$$

We therefore have

$$\mu \equiv \sqrt{1 + \frac{1}{4}\delta^2}$$

Finally, we define the operator D such that

$$Dy(x) = \frac{d}{dx}y(x).$$

To relate D to E, we start with the Taylor's series

$$y(x+h) = y(x) + hy'(x) + \frac{h^2}{2!}y''(x) + \frac{h^3}{3!}y'''(x) + \cdots$$

This can be written in the symbolic form

$$Ey(x) = \left(1 + hD + \frac{h^2D^2}{2!} + \frac{h^3D^3}{3!} + \cdots\right)y(x).$$

Since the series in the brackets is the expansion of e^{hD}, we obtain the interesting result

$$E \equiv e^{hD} \quad \ldots\ldots\ldots\ldots..(3)$$

Using the relation (1), a number of useful identities can be derived. This relation is used to separate the effect of E into that of the powers of Δ and this method of separation is called the method of separation of symbols. The following examples demonstrate the use of this method.

Example 1:

Using the method of separation of symbols, show that

$$\Delta^n u_{x-n} = u_x - nu_{x-1} + \frac{n(n-1)}{2} u_{x-2} + \cdots + (-1)^n u_{x-n}$$

Solution:

To prove this result, we start with the right-hand side. Thus,

$$\begin{aligned}
u_x = nu_{x-1} + \frac{n(n-1)}{2} u_{x-2} + \cdots + (-1)^n u_{x-n} \\
&= u_x - nE^{-1}u_x + \frac{n(n-1)}{2} E^{-2}u_x + \cdots + (-1)^n E^{-n} u_x \\
&= \left[1 - nE^{-1} + \frac{n(n-1)}{2} E^{-2} + \cdots + (-1)^n E^{-n}\right] u_x \\
&= (1 - E^{-1})^n u_x \\
&= \left(1 - \frac{1}{E}\right)^n u_x \\
&= \left(\frac{E-1}{E}\right)^n u_x \\
&= \frac{\Delta^n}{E^n} u_x \\
&= \Delta^n E^{-n} u_x \\
&= \Delta^n u_{x-n}
\end{aligned}$$

which is the left-hand side.

Example 2:

Show that

$$e^x \left(u_0 + x\Delta u_0 + \frac{x^2}{2!}\Delta^2 u_0 + \cdots\right) = u_0 + u_1 x + u_2 \frac{x^2}{2!} + \cdots$$

Solution:

Now,

$$e^x\left(u_0 + x\Delta u_0 + \frac{x^2}{2!}\Delta^2 u_0 + \cdots\right) = e^x\left(1 + x\Delta + \frac{x^2\Delta^2}{2!} + \cdots\right)u_0$$

$$= e^x e^{x\Delta} u_0 = e^{x(1+\Delta)} u_0$$

$$= e^{xE} u_0$$

$$= \left(1 + xE + \frac{x^2E^2}{2!} + \cdots\right)u_0$$

$$= u_0 + xu_1 + \frac{x^2}{2!}u_2 + \cdots$$

which is the required result.

1.4. Detection of Errors by Use of Difference Tables:

Difference tables can be used to check errors in tabular values. Suppose that there is an error of +1 unit in a certain tabular value. As higher differences are formed, the error spreads out fanwise, and is at the same time, considerably magnified, as shown in Table 1.5.

Table 1.5 Detection of Errors using Difference Table

y	Δ	Δ^2	Δ^3	Δ^4	Δ^5
0	0				
0	0	0	0	0	
0	0	0	0	1	1
0	0	1	-3	-4	-5
0	1	-2	3	-10	-10
0	-1	0	0	0	5
0	0	0	0	-1	
0	0	0			
0	0	0			
0	0				

This table shows the following characteristics:

(i) The effect of the error increases with the order of the differences.

(ii) The errors in any one column are the binomial coefficients with alternating signs.

(iii) The algebraic sum of the errors in any difference column is zero, and

(iv) The maximum error occurs opposite the function value containing the error. These facts can be used to detect errors by difference tables. We illustrate this by means of an example.

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*The student should note that Equation (1) does not mean that the operators E and Δ have any existence as separate entities; it merely implies that the effect of the operator E on y_0 is the same as that of the operator $(1 + \Delta)$ on y_0.

Example 3:

Consider the following difference table:

x	y	Δ	Δ^2	Δ^3	Δ^4
1	3010				
2	3424	414	-36		
3	3802	378	-75	+39	+139
4	4105	303	+64	-132	-271
5	4772	297	-68	+49	+181
6	5051	280	-16		-46
7	5315	264			
8					

The term -271 in the fourth difference column has fluctuations of 449 and 452 on either side of it. Comparison with Table 3.5 suggests that there is an error of -45 in the entry for $x = 4$. The correct value of y is therefore $4105 + 45 = 4150$, which shows that the last-two digits have been transposed, a very common form of error. The reader is advised to form a new difference table with this correction, and to check that the third differences are now practically constant.

If an error is present in a given data, the differences of some order will become alternating in sign. Hence, higher-order differences should be formed till the error is revealed as in the above example. If there are errors in several tabular values, then it is not easy to detect the errors by differencing.

1.5 Differences of a Polynomial:

Let $y(x)$ be a polynomial of the nth degree so that

$y(x) = a_0x^n + a_1x^{n-1} + a_2x^{n-2} + \cdots + a_n$. Then we obtain

$$y(x+h) - y(x) = a_0[(x+h)^n - x^n] + a_1[(x+h)^{n-1} - x^{n-1}] + \cdots$$
$$= a_0(nh)x^{n-1} + a_1'x^{n-2} + \cdots + a_n',$$

where $a_1', a_2', \dots, a_n'$ are the new coefficients.

The above equation can be written as

$$\Delta y(x) = a_0(nh)x^{n-1} + a_1'x^{n-2} + \cdots + a_n',$$

which shows that the first difference of a polynomial of the nth degree is a polynomial of degree $(n-1)$. Similarly, the second difference will be a polynomial of degree $(n-2)$, and the coefficient of x^{n-2} will be $a_0n(n-1)h^2$.

Thus the nth difference is $a_0n!\,h^n$, which is a constant. Hence, the $(n+1)$ th, and higher differences of a polynomial of nth degree will be zero. Conversely, if the nth differences of a tabulated function are constant and the $(n+1)$ th, $(n+2)$ th, ..., differences all vanish, then the tabulated function represents a polynomial of degree n. It should be noted that these results hold good only if the values of x are equally spaced. The converse is important in numerical analysis since it enables us to approximate a function by a polynomial if its differences of some order become nearly constant.

Exercises:

1.Form a table of differences for the function $f(x) = x^3 + 5x - 7$ for $x = -1,0,1,2,3,4,5$. Continue the table to obtain $f(6)$ and $f(7)$.

2. Evaluate

(a) $\Delta^2 x^3$

(b) $\Delta^2(\cos x)$

(c) $\Delta[(x+1)(x+2)]$

(d) $\Delta(\tan^{-1} x)$

(e) $\Delta\left[\frac{f(x)}{g(x)}\right]$.

3. Locate and correct the error in the following table:

x	2.5	3.0	3.5	4.0	4.5	5.0	5.5
y	4.32	4.83	5.27	5.47	6.26	6.79	7.23

4. Locate and correct the error in the following table:

x	1.00	1.05	1.10	1.15	1.20	1.25	1.30
e^x	2.7183	2.8577	3.0042	3.1528	3.3201	3.4903	3.6693

5. Prove the following:

(a) $y_x = y_{x-1} + \Delta y_{x-2} + \Delta^2 y_{x-3} + \cdots + \Delta^{n-1} y_{x-n} + \Delta^n y_{x-(n+1)}$

(b) $\Delta^n y_x = y_{x+n} - {}^nC_1 y_{x+n-1} + {}^nC_2 y_{x+n-2} + \cdots + (-1)^n y_x$

(c) $y_1 + y_2 + \cdots + y_n = {}^nC_1 y_1 + {}^nC_2 \Delta y_1 + \cdots + \Delta^{n-1} y_1$

6. From the following table, find the number of students who obtained marks between 60 and 70 :

Marks obtained	$0-40$	$40-60$	$60-80$	$80-100$	$100-120$
No. of students	250	120	100	70	50

7. Find the polynomial which approximates the following values:

x	3	4	5	6	7	8	9
y	13	21	31	43	57	73	91

If the number 31 is the fifth term of the series, find the first and the tenth terms of the series.

8. Find $f(0.23)$ and $f(0.29)$ from the following table:

x	0.20	0.22	0.24	0.26	0.28	0.30
$f(x)$	1.6596	1.6698	1.6804	1.6912	1.7024	1.7139

Unit II

Interpolation: Newton's Interpolation Formulae – Central Difference Interpolation Formulae: Gauss Forward and Backward and Sterling's (only) – Lagrange's Interpolation Formula – Divided Differences– Newton's Divided Differences formula.

Chapter 2: Sections-2.1 to 2.5

2.1. Newton's Formulae for Interpolation:

Given the set of $(n+1)$ values, viz., $(x_0, y_0), (x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, of x and y, it is required to find $y_n(x)$, a polynomial of the nth degree such that y and $y_n(x)$ agree at the tabulated points. Let the values of x be equidistant,

i.e. let $x_i = x_0 + ih, i = 0,1,2, \ldots, n$.

Since $y_n(x)$ is a polynomial of the nth degree, it may be written as

$$\left.\begin{aligned} y_n(x) = \; & a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) \\ & + a_3(x - x_0)(x - x_1)(x - x_2) + \cdots \\ & + a_n(x - x_0)(x - x_1)(x - x_2) \ldots (x - x_{n-1}). \end{aligned}\right\} \ldots\ldots\ldots(1)$$

Imposing now the condition that y and $y_n(x)$ should agree at the set of tabulated points, we obtain

$$a_0 = y_0; a_1 = \frac{y_1 - y_0}{x_1 - x_0} = \frac{\Delta y_0}{h}; a_2 = \frac{\Delta^2 y_0}{h^2 2!}; a_3 = \frac{\Delta^3 y_0}{h^3 3!}; \cdots; a_n = \frac{\Delta^n y_0}{h^n n!};$$

Setting $x = x_0 + ph$ and substituting for $a_0, a_1, \ldots, a_n$, Equation (1) gives

$$y_n(x) = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots + \frac{p(p-1)(p-2)\ldots\ldots(p-n+1)}{n!}\Delta^n y_0$$

$$\ldots\ldots\ldots\ldots..(2)$$

which is Newton's forward difference interpolation formula and is useful for interpolation near the beginning of a set of tabular values.

To find the error committed in replacing the function $y(x)$ by means of the polynomial $y_n(x)$,

$$y(x) - y_n(x) = \frac{(x - x_0)(x - x_1)\ldots(x - x_n)}{(n+1)!} y^{(n+1)}(\xi), x_0 < \xi < x_n \quad \ldots\ldots\ldots. (3)$$

As remarked earlier we do not have any information concerning $y^{(n+1)}(x)$, and therefore, formula given in Equation (3) is useless in practice. Nevertheless, if $y^{(n+1)}(x)$ does not vary too rapidly in the interval, a useful estimate of the derivative can be obtained in the following way. Expanding $y(x+h)$ by Taylor's series theorem, we obtain

$y(x+h) = y(x) + hy'(x) + \frac{h^2}{2!}y''(x) + \cdots$

Neglecting the terms containing h^2 and higher powers of h, this gives

$y'(x) \approx \frac{1}{h}[y(x+h) - y(x)] = \frac{1}{h}\Delta y(x).$

Writing $y'(x)$ as $Dy(x)$ where $D \equiv d/dx$, the differentiation operator, the above equation gives the operator relation

$D \equiv \frac{1}{h}\Delta$ and so $D^{n+1} \equiv \frac{1}{h^{n+1}}\Delta^{n+1}$

We thus obtain $y^{(n+1)}(x) \approx \frac{1}{h^{n+1}}\Delta^{n+1}y(x)$ ……….(4)

Equation (3) can, therefore, be written as

$y(x) - y_n(x) = \frac{p(p-1)(p-2)\ldots(p-n)}{(n+1)!}\Delta^{n+1}y(\xi)$ ………(5)

in which form it is suitable for computation.

Instead of assuming $y_n(x)$ as in Equation (1), if we choose it in the form

$$\begin{aligned} y_n(x) =& a_0 + a_1(x-x_n) + a_2(x-x_n)(x-x_{n-1}) \\ &+ a_3(x-x_n)(x-x_{n-1})(x-x_{n-2}) + \cdots \\ &+ a_n(x-x_n)(x-x_{n-1})\ldots(x-x_1) \end{aligned}$$

and then impose the condition that y and $y_n(x)$ should agree at the tabulated points $x_n, x_{n-1}, \ldots, x_2, x_1, x_0$, we obtain (after some simplification)

$$y_n(x) = y_n + p\nabla y_n + \frac{p(p+1)}{2!}\nabla^2 y_n + \cdots + \frac{p(p+1)\ldots(p+n-1)}{n!}\nabla^n y_n \ldots\ldots\ldots (6)$$

where $p = (x - x_n)/h$.

This is Newton's backward difference interpolation formula and it uses tabular values to the left of y_n. This formula is therefore useful for interpolation near the end of the tabular values.

It can be shown that the error in this formula may be written as

$y(x) - y_n(x) = \frac{p(p+1)(p+2)\ldots(p+n)}{(n+1)!}\nabla^{n+1}y(\xi)$ ……….(7)

where $x_0 < x < x_n$ and $x = x_n + ph$.

The following examples illustrate the use of these formulae.

Example 1:

Find the cubic polynomial which takes the following values:

$y(1) = 24, y(3) = 120, y(5) = 336$, and $y(7) = 720$. Hence, or otherwise, obtain the value of $y(8)$.

Solution:

We form the difference table:

x	y	Δ	Δ^2	Δ^3
1	24			
		96		
3	120		120	
		216		48
5	336		168	
		384		
7	720			

Here $h = 2$. With $x_0 = 1$, we have $x = 1 + 2p$ or $p = (x - 1)/2$. Substituting this value of p in equation (2), we obtain

$$y(x) = 24 + \frac{x-1}{2}(96) + \frac{\left(\frac{x-1}{2}\right)\left(\frac{x-1}{2}-1\right)}{2}(120) + \frac{\left(\frac{x-1}{2}\right)\left(\frac{x-1}{2}-1\right)\left(\frac{x-1}{2}-2\right)}{6}(48)$$
$$= x^3 + 6x^2 + 11x + 6.$$

To determine $y(8)$, we observe that $p = 7/2$. Hence, Eq. (3.10) gives:

$$y(8) = 24 + \frac{7}{2}(96) + \frac{(7/2)(7/2-1)}{2}(120) + \frac{(7/2)(7/2-1)(7/2-2)}{6}(48) = 990.$$

Direct substitution in $y(x)$ also yields the same value.

Note:

This process of finding the value of y for some value of x outside the given range is called extrapolation and this example demonstrates the fact that if a tabulated function is a polynomial, then both interpolation and extrapolation would give exact values.

Example 2:

Using Newton's forward difference formula, find the sum

$S_n = 1^3 + 2^3 + 3^3 + \cdots + n^3$

We have

$S_{n+1} = 1^3 + 2^3 + 3^3 + \cdots + n^3 + (n+1)^3$

Hence

$S_{n+1} - S_n = (n+1)^3$

or $\Delta S_n = (n+1)^3$

Solution:

It follows that

$$\Delta^2 S_n = \Delta S_{n+1} - \Delta S_n = (n+2)^3 - (n+1)^3 = 3n^2 + 9n + 7$$
$$\Delta^3 S_n = 3(n+1)^2 + 9n + 7 - (3n^2 + 9n + 7) = 6n + 12$$
$$\Delta^4 S_n = 6(n+1) + 12 - (6n + 12) = 6$$

Since $\Delta^5 S_n = \Delta^6 S_n = \cdots = 0, S_n$ is a fourth-degree polynomial in n.

Further,

$S_1 = 1, \Delta S_1 = 8, \Delta^2 S_1 = 19, \Delta^3 S_1 = 18, \Delta^4 S_1 = 6$

Equation (2) gives

$$S_n = 1 + (n-1)(8) + \frac{(n-1)(n-2)}{2}(19) + \frac{(n-1)(n-2)(n-3)}{6}(18)$$
$$+ \frac{(n-1)(n-2)(n-3)(n-4)}{24}(6)$$
$$= \frac{1}{4}n^4 + \frac{1}{2}n^3 + \frac{1}{4}n^2$$
$$= \left[\frac{n(n+1)}{2}\right]^2.$$

Example 3:

Values of x (in degrees) and $\sin x$ are given in the following table:

x (in degrees)	$\sin x$
15	0.2588190
20	0.3420201
25	0.4226183
30	0.5
35	0.5735764
40	0.6427876

Determine the value of $\sin 38°$.

The difference table is

The difference table is

x	$\sin x$	Δ	Δ^2	Δ^3	Δ^4	Δ^5
15	0.2588190					
		0.0832011				
20	0.3420201		−0.0026029			
		0.0805982		−0.0006136		
25	0.4226183		−0.0032165		0.0000248	
		0.0773817		−0.0005888		0.0000041
30	0.5		−0.0038053		0.0000289	
		0.0735764		−0.0005599		
35	0.5735764		−0.0043652			
		0.0692112				
40	0.6427876					

To find sin 38°, we use Newton's backward difference formula with $x_n = 40$ and $x = 38$. This gives

$p = \frac{x-x_n}{h} = \frac{38-40}{5} = -\frac{2}{5} = -0.4.$

Hence, using Equation (6), we obtain

$$
\begin{aligned}
y(38) =& 0.6427876 - 0.4(0.0692112) + \frac{-0.4(-0.4+1)}{2}(-0.0043652) \\
&+ \frac{(-0.4)(-0.4+1)(-0.4+2)}{6}(-0.0005599) \\
&+ \frac{(-0.4)(-0.4+1)(-0.4+2)(-0.4+3)}{24}(0.0000289) \\
&+ \frac{(-0.4)(-0.4+1)(-0.4+2)(-0.4+3)(-0.4+4)}{120}(0.0000041) \\
=& 0.6427876 - 0.02768448 + 0.00052382 + 0.00003583 - 0.00000120 \\
=& 0.6156614.
\end{aligned}
$$

Example 4:

Find the missing term in the following table:

x	y
0	1
1	3
2	9
3	-
4	81

Explain why the result differs from $3^3 = 27$.

Solution:

Since four points are given, the given data can be approximated by a third-degree polynomial in x. Hence $\Delta^4 y_0 = 0$. Substituting $\Delta = E - 1$ and simplifying, we get

$E^4 y_0 - 4E^3 y_0 + 6E^2 y_0 - 4E y_0 + y_0 = 0$

Since $E^r y_0 = y_r$, the above equation becomes

$y_4 - 4y_3 + 6y_2 - 4y_1 + y_0 = 0$

Substituting for y_0, y_1, y_2 and y_4 in the above, we obtain

$y_3 = 31$

The tabulated function is 3^x and the exact value of $y(3)$ is 27 . The error is due to the fact that the exponential function 3^x is approximated by means of a polynomial in x of degree 3.

Example 5:

The table below gives the values of $\tan x$ for $0.10 \leq x \leq 0.30$:

x	$y = \tan x$
0.10	0.1003
0.15	0.1511
0.20	0.2027
0.25	0.2553
0.30	0.3093

Find : (a) tan 0.12 (b) tan 0.26, (c) tan 0.40 and (d) tan 0.50.

The table of difference is

x	y	Δ	Δ^2	Δ^3	Δ^4
0.10	0.1003				
		0.0508			
0.15	0.1511		0.0008		
		0.0516		0.0002	
0.20	0.2027		0.0010		0.0002
		0.0526		0.0004	
0.25	0.2553		0.0014		
		0.0540			
0.30	0.3093				

(a) To find $\tan(0.12)$, we have $0.12 = 0.10 + p(0.05)$, which gives $p = 0.4$. Hence, equation(2) gives

$$\tan(0.12) = 0.1003 + 0.4(0.0508) + \frac{0.4(0.4-1)}{2}(0.0008) + \frac{0.4(0.4-1)(0.4-2)}{6}(0.0002) + \frac{0.4(0.4-1)(0.4-2)(0.4-3)}{24}(0.0002) = 0.1205.$$

(b) To find $\tan(0.26)$, we have $0.26 = 0.30 + p(0.05)$, which gives $p = -0.8$. Hence, Equation (6) gives

$$\tan(0.26) = 0.3093 - 0.8(0.0540) + \frac{-0.8(-0.8+1)}{2}(0.0014) + \frac{-0.8(-0.8+1)(-0.8+2)}{6}(0.0004) + \frac{-0.8(-0.8+1)(-0.8+2)(-0.8+3)}{24}(0.0002) = 0.2662$$

Proceeding as in the case (i) above, we obtain

(c) $\tan(0.40) = 0.4241$, and

(d) $\tan(0.50) = 0.5543$.

The actual values, correct to four decimal places, of $\tan(0.12)$, $\tan(0.26)$, $\tan(0.40)$ and $\tan(0.50)$ are respectively 0.1206, 0.2660, 0.4228 and 0.5463. Comparison of the computed and actual values shows that in the first-two cases (i.e. of interpolation) the results obtained are fairly accurate whereas in the last-two cases (i.e. of extrapolation) the errors are quite considerable. The example therefore demonstrates the important result that if a tabulated function is other than a polynomial, then extrapolation very far from the table limits would be dangerous-although interpolation can be carried out very accurately.

2.2. Central Difference Interpolation Formulae:

In the preceding section, we derived and discussed Newton's forward and backward interpolation formulae, which are applicable for interpolation near the beginning and end respectively, of tabulated values. We shall, in the present section, discuss the central difference formulae which are most suited for interpolation near the middle of a tabulated set. The central difference operator δ was already introduced in Section 1.3.3.

The most important central difference formulae are those due to Stirling, Bessel and Everett. These will be discussed in Sections 2.2.2, 2.2.3 and 2.2.4, respectively. Gauss's formulae, introduced in Section 2.2.1 below, are of interest from a theoretical stand-point only.

2.2.1. Gauss' Central Difference Formulae:

In this section, we will discuss Gauss' forward and backward formulae.

Gauss' forward formula

We consider the following difference table in which the central ordinate is taken for convenience as y_0 corresponding to $x = x_0$.

The differences used in this formula lie on the line shown in Table 3.6. The formula is, therefore, of the form

$y_p = y_0 + G_1 \Delta y_0 + G_2 \Delta^2 y_{-1} + G_3 \Delta^3 y_{-1} + G_4 \Delta^4 y_{-2} + \cdots$ ....(1)

where $G_1, G_2, \ldots$ have to be determined. The y_p on the left side can be expressed in terms of $y_0, \Delta y_0$ and higher-order differences of y_0, as follows:

Table 2.1. Gauss' Forward Formula

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
x_{-3}	y_{-3}						
		Δy_{-3}					
x_{-2}	y_{-2}		$\Delta^2 y_{-3}$				
		Δy_{-2}		$\Delta^3 y_{-3}$			
x_{-1}	y_{-1}		$\Delta^2 y_{-2}$		$\Delta^4 y_{-3}$		
		Δy_{-1}		$\Delta^3 y_{-2}$		$\Delta^5 y_{-3}$	
x_0	y_0		$\Delta^2 y_{-1}$		$\Delta^4 y_{-2}$		$\Delta^6 y_{-3}$
		Δy_0		$\Delta^3 y_{-1}$		$\Delta^5 y_{-2}$	
x_1	y_1		$\Delta^2 y_0$		$\Delta^4 y_{-1}$		
		Δy_1		$\Delta^3 y_0$			
x_2	y_2		$\Delta^2 y_1$				
		Δy_2					
x_3	y_3						

$$y_p = E^p y_0$$

Clearly, $= (1+\Delta)^p y_0$, using relation equation(1)

$$= y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots$$

Similarly, the right side of Equation (1) can also be expressed in terms of $y_0, \Delta y_0$ and higher-order differences. We have

$$\begin{aligned}\Delta^2 y_{-1} &= \Delta^2 E^{-1} y_0\\ &= \Delta^2(1+\Delta)^{-1} y_0\\ &= \Delta^2(1-\Delta+\Delta^2-\Delta^3+\cdots)y_0\\ &= \Delta^2(y_0-\Delta y_0+\Delta^2 y_0-\Delta^3 y_0+\cdots)\\ &= \Delta^2 y_0-\Delta^3 y_0+\Delta^4 y_0-\Delta^5 y_0+\cdots\end{aligned}$$

$$\Delta^3 y_{-1} = \Delta^3 y_0-\Delta^4 y_0+\Delta^5 y_0-\Delta^6 y_0+\cdots$$

$$\begin{aligned}\Delta^4 y_{-2} &= \Delta^4 E^{-2} y_0\\ &= \Delta^4(1+\Delta)^{-2} y_0\\ &= \Delta^4(y_0-2\Delta y_0+3\Delta^2 y_0-4\Delta^3 y_0+\cdots)\\ &= \Delta^4 y_0-2\Delta^5 y_0+3\Delta^6 y_0-4\Delta^7 y_0+\cdots\end{aligned}$$

Hence Equation (1) gives the identity

$$\begin{aligned}&y_0+p\Delta y_0+\frac{p(p-1)}{2!}\Delta^2 y_0+\frac{p(p-1)(p-2)}{3!}\Delta^3 y_0\\ &\quad+\frac{p(p-1)(p-2)(p-3)}{4!}\Delta^4 y_0+\cdots\\ &=y_0+G_1\Delta y_0+G_2(\Delta^2 y_0-\Delta^3 y_0+\Delta^4 y_0-\Delta^5 y_0+\cdots)\\ &\quad+G_3(\Delta^3 y_0-\Delta^4 y_0+\Delta^5 y_0-\Delta^6 y_0+\cdots)\\ &\quad+G_4(\Delta^4 y_0-2\Delta^5 y_0+3\Delta^6 y_0-4\Delta^7 y_0+\cdots) \ \ldots\ldots\ldots (2)\end{aligned}$$

Equating the coefficients of $\Delta y_0, \Delta^2 y_0, \Delta^3 y_0$, etc., on both sides of equation (2), we obtain

$$\begin{aligned}G_1 &= p\\ G_2 &= \frac{p(p-1)}{2!}, G_3 = \frac{(p+1)p(p-1)}{3!} \qquad \ldots\ldots\ldots\ldots (3)\\ G_4 &= \frac{(p+1)p(p-1)(p-2)}{4!}\end{aligned}$$

Gauss' backward formula

This formula uses the differences which lie on the line shown in Table 2.2.

Table 2.2 Gauss' Backward Formula

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
⋮	⋮						
x_{-1}	y_{-1}						
		Δy_{-1}		$\Delta^3 y_{-2}$		$\Delta^5 y_{-3}$	
x_0	y_0		$\Delta^2 y_{-1}$		$\Delta^4 y_{-2}$		$\Delta^6 y_{-3}$
		Δy_0		$\Delta^3 y_{-1}$		$\Delta^5 y_{-2}$	
x_1	y_1						
⋮	⋮						

Gauss' backward formula can therefore be assumed to be of the form

$$y_p = y_0 + G_1'\Delta y_{-1} + G_2'\Delta^2 y_{-1} + G_3'\Delta^3 y_{-2} + G_4'\Delta^4 y_{-2} + \cdots (4)$$

where $G_1', G_2', \ldots$ have to be determined. Following the same procedure as in Gauss' forward formula, we obtain

$$\left.\begin{aligned} G_1' &= p \\ G_2' &= \frac{p(p+1)}{2!}, \\ G_3' &= \frac{(p+1)p(p-1)}{3!} \\ G_4' &= \frac{(p+2)(p+1)p(p-1)}{4!} \\ &\vdots \end{aligned}\right\} \ldots\ldots\ldots\ldots (5)$$

Example 1:

From the following table, find the value of $e^{1.17}$ using Gauss' forward formula:

x	e^x
1.00	2.7183
1.05	2.8577
1.10	3.0042
1.15	3.1582
1.20	3.3201
1.25	3.4903
1.30	3.6693

We have

$1.17 = 1.15 + p(0.05)$

which gives

$p = \frac{0.02}{0.05} = \frac{1}{4}.$

The difference table is given below.

x	e^x	Δ	Δ^2	Δ^3	Δ^4
1.00	2.7183				
		0.1394			
1.05	2.8577		0.0071		
		0.1465		0.0004	
1.10	3.0042		0.0075		0
		0.1540		0.0004	
1.15	3.1582		0.0079		0
		0.1619		0.0004	
1.20	3.3201		0.0083		0.0001
		0.1702		0.0005	
1.25	3.4903		0.0088		
		0.1790			
1.30	3.6693				

Using formulae (1) and (3), we obtain

$$e^{1.17} = 3.1582 + \frac{2}{5}(0.1619) + \frac{(2/5)(2/5-1)}{2}(0.0079) + \frac{(2/5+1)(2/5)(2/5-1)}{6}(0.0004)$$
$$= 3.1582 + 0.0648 - 0.0009$$
$$= 3.2221$$

2.2.2 Stirling's Formula:

Taking the mean of Gauss' forward and backward formulae, we obtain

$$y_p = y_0 + p\frac{\Delta y_{-1} + \Delta y_0}{2} + \frac{p^2}{2}\Delta^2 y_{-1} + \frac{p(p^2-1)}{3!}\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2} \quad \ldots\ldots\ldots(6)$$

Formula given in Equation (6) is called Stirling's formula.

2.3. Lagrange's Interpolation Formula:

Let $y(x)$ be continuous and differentiable $(n+1)$ times in the interval (a, b). Given the $(n+1)$ points $(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)$ where the values of x need not necessarily be equally spaced, we wish to find a polynomial of degree n, say $L_n(x)$, such that

$L_n(x_i) = y(x_i) = y_i, i = 0,1, \ldots, n$ ……….(1)

Before deriving the general formula, we first consider a simpler case, viz., the equation of a straight line (a linear polynomial) passing through two points (x_0, y_0) and (x_1, y_1). Such a polynomial, say $L_1(x)$, is easily seen to be

$$L_1(x) = \frac{x - x_1}{x_0 - x_1} y_0 + \frac{x - x_0}{x_1 - x_0} y_1$$
$$= l_0(x) y_0 + l_1(x) y_1 = \sum_{i=0}^{1} l_i(x) y_i \ldots\ldots\ldots (2)$$

where $l_0(x) = \frac{x - x_1}{x_0 - x_1}$ and $l_1(x) = \frac{x - x_0}{x_1 - x_0}$ ………..(3)

From Equation (1), it is seen that

$l_0(x_0) = 1, l_0(x_1) = 0, l_1(x_0) = 0, l_1(x_1) = 1.$

These relations can be expressed in a more convenient form as

$$l_i(x_j) = \begin{cases} 1, \text{ if } i = j \\ 0, \text{ if } i \neq j \end{cases} \ldots\ldots\ldots (4)$$

The $l_i(x)$ in Equation (2) also have the property

$$\sum_{i=0}^{1} l_i(x) = l_0(x) + l_1(x) = \frac{x - x_1}{x_0 - x_1} + \frac{x - x_0}{x_1 - x_0} = 1 \ldots\ldots\ldots(5)$$

Equation (2) is the Lagrange polynomial of degree one passing through two points (x_0, y_0) and (x_1, y_1). In a similar way, the Lagrange polynomial of degree two passing through three points $(x_0, y_0), (x_1, y_1)$ and (x_2, y_2) is written as

$$L_2(x) = \sum_{i=0}^{2} l_i(x) y_i$$

where the $l_i(x)$ satisfy the conditions given in Equations. (4) and (5).

To derive the general formula, let $L_n(x) = a_0 + a_1x + a_2x^2 + \cdots + a_nx^n$ ....(6) be the desired polynomial of the nth degree such that conditions given in Equation (1) (called the interpolatory conditions) are satisfied. Substituting these conditions in Eq. (6), we obtain the system of equations

$$\left.\begin{aligned} y_0 &= a_0 + a_1x_0 + a_2x_0^2 + \cdots + a_nx_0^n \\ y_1 &= a_0 + a_1x_1 + a_2x_1^2 + \cdots + a_nx_1^n \\ y_2 &= a_0 + a_1x_2 + a_2x_2^2 + \cdots + a_nx_2^n \\ &\vdots \\ y_n &= a_0 + a_1x_n + a_2x_n^2 + \cdots + a_nx_n^n \end{aligned}\right\} \quad ....(7)$$

The set of Equations. (7) will have a solution if $\begin{vmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{vmatrix} \neq 0$ ....(8)

The value of this determinant, called Vandermonde's determinant, is

$(x_0 - x_1)(x_0 - x_2) \ldots (x_0 - x_n)(x_1 - x_2) \ldots (x_1 - x_n) \ldots (x_{n-1} - x_n)$.

Eliminating $a_0, a_1, \ldots, a_n$ from Equations. (6) and (7), we obtain

$$\begin{vmatrix} L_n(x) & 1 & x & x^2 & \cdots & x^n \\ y_0 & 1 & x_0 & x_0^2 & \cdots & x_0^n \\ y_1 & 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ y_n & 1 & x_n & x_n^2 & \cdots & x_n^n \end{vmatrix} = 0 \quad ....(9)$$

which shows that $L_n(x)$ is a linear combination of $y_0, y_1, y_2, \ldots, y_n$. Hence we write

$L_n(x) = \sum_{i=0}^{n} l_i(x)y_i$ ....(10)

where $l_i(x)$ are polynomials in x of degree n. Since $L_n(x_j) = y_j$ for $j = 0,1,2,\ldots,n$, Equation (5) gives

$$\left.\begin{aligned} l_i(x_j) &= 0 \quad \text{if } i \neq j \\ l_j(x_j) &= 1 \quad \text{for all } j \end{aligned}\right\}$$

which are the same as Equation(4). Hence $l_i(x)$ may be written as

$$l_i(x) = \frac{(x-x_0)(x-x_1)\ldots(x-x_{i-1})(x-x_{i+1})\ldots(x-x_n)}{(x_i-x_0)(x_i-x_1)\ldots(x_i-x_{i-1})(x_i-x_{i+1})\ldots(x_i-x_n)} \quad ....(11)$$

which obviously satisfies the conditions (4).

If we now set

$$\Pi_{n+1}(x) = (x - x_0)(x - x_1) \ldots (x - x_{i-1})(x - x_i)(x - x_{i+1}) \ldots (x - x_n) \quad ....(12)$$

then

$\Pi'_{n+1}(x_i) = \frac{d}{dx}[\Pi_{n+1}(x)]_{X=x_i}$

so that Equation (11) becomes $l_i(x) = \frac{\Pi_{n+1}(x)}{(x-x_i)\Pi'_{n+1}(x_i)}$ ………… (13)

Hence Equation (10) gives $L_n(x) = \sum_{i=0}^{n} \frac{\Pi_{n+1}(x)}{(x-x_i)\Pi'_{n+1}(x_i)} y_i$ ………. (14)

which is called Lagrange's interpolation formula. The coefficients $l_i(x)$, defined in Eq. (11), are called Lagrange interpolation coefficients. Interchanging x and y in Equation (14), we obtain the formula $L_n(y) = \sum_{i=0}^{n} \frac{\Pi_{n+1}(y)}{(y-y_i)\Pi'_{n+1}(y_i)} x_i$ ……… (15)

which is useful for inverse interpolation.

It is trivial to show that the Lagrange interpolating polynomial is unique. To prove this, we assume the contrary. Let $\bar{L}_n(x)$ be a polynomial, distinct from $L_n(x)$, of degree not exceeding n and such that

$\bar{L}_n(x_i) = y_i, i = 0,1,2, \dots, n$

Then the polynomial defined by $M(x)$, where

$M(x) = L_n(x) - \bar{L}_n(x)$

vanishes at the $(n+1)$ points $x_i, i = 0,1, \dots, n$. Hence we have

$M_n(x) \equiv 0,$

which shows that $L_n(x)$ and $\bar{L}_n(x)$ are identical.

A major advantage of this formula is that the coefficients in Equation (15) are easily determined. Further, it is more general in that it is applicable to either equal or unequal intervals and the abscissae $x_0, x_1, \dots, x_n$ need not be in order. Using this formula it is, however, inconvenient to pass from one interpolation polynomial to another of degree one greater.

The following examples illustrate the use of Lagrange's formula.

Example 1:

Certain corresponding values of x and $\log_{10} x$ are

$(300,2.4771), (304,2.4829), (305,2.4843)$ and $(307,2.4871)$. Find $\log_{10} 301$.

From formula given in Eq. (14), we obtain

$$\log_{10} 301 = \frac{(-3)(-4)(-6)}{(-4)(-5)(-7)}(2.4771) + \frac{(1)(-4)(-6)}{(4)(-1)(-3)}(2.4829)$$
$$+ \frac{(1)(-3)(-6)}{(5)(1)(-2)}(2.4843) + \frac{(1)(-3)(-4)}{(7)(3)(2)}(2.4871)$$
$$= 1.2739 + 4.9658 - 4.4717 + 0.7106$$
$$= 2.4786.$$

Example 2:

If $y_1 = 4, y_3 = 12, y_4 = 19$ and $y_x = 7$, find x.

Using Equation (15), we have

$$x = \frac{(-5)(-12)}{(-8)(-15)}(1) + \frac{(3)(-12)}{(8)(-7)}(3) + \frac{(3)(-5)}{(15)(7)}(4)$$
$$= \frac{1}{2} + \frac{27}{14} - \frac{4}{7}$$
$$= 1.86.$$

The actual value is 2.0 since the above values were obtained from the polynomial $y(x) = x^2 + 3$.

Example 3:

Find the Lagrange interpolating polynomial of degree 2 approximating the function $y = \ln x$ defined by the following table of values. Hence determine the value of $\ln 2.7$.

x	$y = \ln x$
2	0.69315
2.5	0.91629
3.0	1.09861

We have

$$l_0(x) = \frac{(x-2.5)(x-3.0)}{(-0.5)(-1.0)} = 2x^2 - 11x + 15$$

Similarly, we find

$l_1(x) = -(4x^2 - 20x + 24)$ and $l_2(x) = 2x^2 - 9x + 10.$

Hence

$$L_2(x) = (2x^2 - 11x + 15)(0.69315) - (4x^2 - 20x + 24)(0.91629)$$
$$+(2x^2 - 9x + 10)(1.09861)$$
$$= -0.08164x^2 + 0.81366x - 0.60761,$$

which is the required quadratic polynomial.

Putting $x = 2.7$, in the above polynomial, we obtain

$\ln 2.7 \approx L_2(2.7) = -0.08164(2.7)^2 + 0.81366(2.7) - 0.60761 = 0.9941164.$

Actual value of $\ln 2.7 = 0.9932518$, so that

$|\text{ Error } | = 0.0008646.$

Example 4:

The function $y = \sin x$ is tabulated below

x	$y = \sin x$
0	0
$\pi/4$	0.70711
$\pi/2$	1.0

Using Lagrange's interpolation formula, find the value of $\sin(\pi/6)$.

We have

$$\sin\frac{\pi}{6} \approx \frac{(\pi/6-0)(\pi/6-\pi/2)}{(\pi/4-0)(\pi/4-\pi/2)}(0.70711) + \frac{(\pi/6-0)(\pi/6-\pi/4)}{(\pi/2-0)(\pi/2-\pi/4)}(1)$$

$$= \frac{8}{9}(0.70711) - \frac{1}{9}$$

$$= \frac{4.65688}{9}$$

$$= 0.51743$$

Example 5:

Using Lagrange's interpolation formula, find the form of the function $y(x)$ from the following table

x	y
0	-12
1	0
3	12
4	24

Since $y = 0$ when $x = 1$, it follows that $x - 1$ is a factor. Let $y(x) = (x-1)R(x)$. Then $R(x) = y/(x-1)$. We now tabulate the values of x and $R(x)$.

x	$R(x)$
0	12
3	6
4	8

Applying Lagrange's formula to the above table, we find

$$R(x) = \frac{(x-3)(x-4)}{(-3)(-4)}(12) + \frac{(x-0)(x-4)}{(3-0)(3-4)}(6) + \frac{(x-0)(x-3)}{(4-0)(4-3)}(8)$$
$$= (x-3)(x-4) - 2x(x-4) + 2x(x-3)$$
$$= x^2 - 5x + 12.$$

Hence the required polynomial approximation to $y(x)$ is given by

$$y(x) = (x-1)(x^2 - 5x + 12)$$

2.3.1. Error in Lagrange's Interpolation Formula:

Equation (3.7) can be used to estimate the error of the Lagrange interpolation formula for the class of functions which have continuous derivatives of order up to $(n+1)$ on $[a,b]$. We, therefore, have

$$y(x) - L_n(x) = R_n(x) = \frac{\Pi_{n+1}(x)}{(n+1)!} y^{(n+1)}(\xi), a < \xi < b \quad \text{.......... (1)}$$

and the quantity E_L, where $E_L = \max_{[a,b]} |R_n(x)|$ .... (2)

may be taken as an estimate of error. Further, if we assume that

$$\left|y^{(n+1)}(\xi)\right| \leq M_{n+1}, a \leq \xi \leq b \quad \text{..........(3)}$$

then $E_L \leq \frac{M_{n+1}}{(n+1)!} \max_{[a,b]} |\Pi_{n+1}(x)|$ ....(4)

The following examples illustrate the computation of the error.

Example 1:

Estimate the error in the value of y obtained in Example 3.15.

Since $y = \ln x$, we obtain $y' = 1/x, y'' = -1/x^2$ and $y''' = 2/x^3$. It follows that $y'''(\xi) = 2/\xi^3$. Thus the continuity conditions on $y(x)$ and its derivatives are satisfied in $[2,3]$. Hence $R_n(x) = \frac{(x-2)(x-2.5)(x-3)}{6} \frac{2}{\xi^3}, 2 < \xi < 3$ But $\left|\frac{1}{\xi^3}\right| < \frac{1}{2^3} = \frac{1}{8}$

When $x = 2.7$, we therefore obtain

$$|R_n(x)| \leq \left|\frac{(2.7-2)(2.7-2.5)(2.7-3)}{6} \frac{2}{8}\right| = \frac{0.7 \times 0.2 \times 0.3}{3 \times 8} = 0.00175$$

which agrees with the actual error given in Example 3.15.

Example 2:

Estimate the error in the solution computed in Example 3.16.

Since $y(x) = \sin x$, we have

$$y'(x) = \cos x, y''(x) = -\sin x, y'''(x) = -\cos x$$

Hence $|y'''(\xi)| < 1$.

When $x = \pi/6$.

$$|R_n(x)| \leq \left|\frac{(\pi/6-0)(\pi/6-\pi/4)(\pi/6-\pi/2)}{6}\right| = \frac{1}{6}\frac{\pi}{6}\frac{\pi}{12}\frac{\pi}{3} = 0.02392$$

which agrees with the actual error in the solution obtained in Example 3.16.

2.4. Divided differences and their properties:

The Lagrange interpolation formula, derived in Section 3.9.1, has the disadvantage that if another interpolation point were added, then the interpolation coefficients $l_i(x)$ will have to be recomputed. We therefore seek an interpolation polynomial which has the property that a polynomial of higher degree may be derived from it by simply adding new terms. Newton's general interpolation formula is one such formula and it employs what are called divided differences. It is our principal purpose in this section to define such differences and discuss certain of their properties to obtain the basic formula due to Newton.

Let $(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n)$ be the given $(n+1)$ points. Then the divided differences of order $1, 2, \dots, n$ are defined by the relations:

$$\left.\begin{aligned} [x_0, x_1] &= \frac{y_1 - y_0}{x_1 - x_0}, \\ [x_0, x_1, x_2] &= \frac{[x_1, x_2] - [x_0, x_1]}{x_2 - x_0}, \\ &\vdots \\ [x_0, x_1, \dots, x_n] &= \frac{[x_1, x_2, \dots, x_n] - [x_0, x_1, \dots, x_{n-1}]}{x_n - x_0}. \end{aligned}\right\} \dots\dots\dots (1)$$

Even if the arguments are equal, the divided differences may still have a meaning. We then set $x_1 = x_0 + \varepsilon$ so that

$$\begin{aligned} [x_0, x_1] &= \lim_{\varepsilon \to 0} [x_0, x_0 + \varepsilon] \\ &= \lim_{\varepsilon \to 0} \frac{y(x_0 + \varepsilon) - y(x_0)}{\varepsilon} \\ &= y'(x_0), \text{ if } y(x) \text{ is differentiable.} \end{aligned}$$

Similarly, $\underbrace{[x_0, x_0, \dots, x_0]}_{(r+1) \text{ arguments}} = \frac{y^r(x_0)}{r!}$ ....(2)

From Equation (2), it is easy to see that

$$[x_0, x_1] = \frac{y_0}{x_0 - x_1} + \frac{y_1}{x_1 - x_0} = [x_1, x_0].$$

Again,

$$\begin{aligned} [x_0, x_1, x_2] &= \frac{1}{x_2 - x_0}\left(\frac{y_2 - y_1}{x_2 - x_1} - \frac{y_1 - y_0}{x_1 - x_0}\right) \\ &= \frac{1}{x_2 - x_0}\left[\frac{y_2}{x_2 - x_1} - y_1\left(\frac{1}{x_2 - x_1} + \frac{1}{x_1 - x_0}\right) + \frac{y_0}{x_1 - x_0}\right] \\ &= \frac{y_0}{(x_0 - x_1)(x_0 - x_2)} + \frac{y_1}{(x_1 - x_0)(x_1 - x_2)} + \frac{y_2}{(x_2 - x_0)(x_2 - x_1)} \dots\dots\dots (3) \end{aligned}$$

Similarly it can be shown that

$$[x_0, x_1, \dots, x_n] = \frac{y_0}{(x_0 - x_1)\dots(x_0 - x_n)} + \frac{y_1}{(x_1 - x_0)\dots(x_1 - x_n)} + \dots \frac{y_n}{(x_n - x_0)(x_n - x_{n-1})} \dots\dots(4)$$

Hence the divided differences are symmetrical in their arguments.

Now let the arguments be equally spaced so that $x_1 - x_0 = x_2 - x_1 = \cdots = x_n - x_{n-1} = h$. Then we obtain $[x_0, x_1] = \frac{y_1 - y_0}{x_1 - x_0} = \frac{1}{h}\Delta y_0$ ....(5)

$[x_0, x_1, x_2] = \frac{[x_1, x_2] - [x_0, x_1]}{x_2 - x_0} = \frac{1}{2h}\left(\frac{\Delta y_1}{h} - \frac{\Delta y_0}{h}\right) = \frac{1}{2h^2}\Delta^2 y_0 = \frac{1}{h^2 2!}\Delta^2 y_0$ ....(6)

and in general, $[x_0, x_1, \dots, x_n] = \frac{1}{h^n n!}\Delta^n y_0$ ....(7)

If the tabulated function is a polynomial of nth degree, then $\Delta^n y_0$ would be a constant and hence the nth divided difference would also be a constant.

For the set of values $(x_i, y_i), i = 0,1,2, \dots, n$, divided differences can be generated by the following statements.

```
Define y (xj) = yj = DD (0, j), j = 0, 1, 2, .., n
Do i = 1(1)n
Do j = O(1)(n-i)
DD(i, j) = (DD(i-1, j+1) - DD(i-1, j)) / (X(i+j) - X(j))
Next j
Next i
```

2.5. Newton's General Interpolation Formula:

By definition, we have

$[x, x_0] = \frac{y - y_0}{x - x_0}$

so that $y = y_0 + (x - x_0)[x, x_0]$ .... (1)

Again

$[x, x_0, x_1] = \frac{[x, x_0] - [x_0, x_1]}{x - x_1}$

which gives

$[x, x_0] = [x_0, x_1] + (x - x_1)[x, x_0, x_1]$

Substituting this value of $[x, x_0]$ in Equation (1), we obtain

$y = y_0 + (x - x_0)[x_0, x_1] + (x - x_0)(x - x_1)[x, x_0, x_1]$ ....(2)

But

$[x, x_0, x_1, x_2] = \frac{[x, x_0, x_1] - [x_0, x_1, x_2]}{x - x_2}$

and so $[x, x_0, x_1] = [x_0, x_1, x_2] + (x - x_2)[x, x_0, x_1, x_2]$ ....(3)

Equation (2) now gives

$$y = y_0 + (x - x_0)[x_0, x_1] + (x - x_0)(x - x_1)[x_0, x_1, x_2]$$
$$+ (x - x_0)(x - x_1)(x - x_2)[x, x_0, x_1, x_2] \quad \ldots\ldots\ldots\ldots(4)$$

Proceeding in this way, we obtain

$$y = y_0 + (x - x_0)[x_0, x_1] + (x - x_0)(x - x_1)[x_0, x_1, x_2]$$
$$+ (x - x_0)(x - x_1)(x - x_2)[x_0, x_1, x_2, x_3] + \cdots$$
$$+ (x - x_0)(x - x_1)(x - x_2) \ldots\ldots (x - x_n)[x_0, x_1, x_2, x_3 \ldots\ldots x_n] \quad \ldots\ldots\ldots(5)$$

This formula is called Newton's general interpolation formula with divided differences, the last term being the remainder term after ($n + 1$) terms.

After generating the divided differences, interpolation can be carried out by the following statements.

Let y_k be required corresponding to the value $x = x_k$. Then

$y_k = y_0$

factor = 1.0

Do i = 0(1) (n-1)

factor = factor * $(x_k - x_i)$

$Y_k = Y_k +$ factor * DD (i+1,0)

Next i

End

Example 1:

As our first example to illustrate the use of Newton's divided difference formula, we consider the data of (Example 1 of section 2.3).

The divided difference table is

x	$\log_{10} x$		
300	2.4771	0.00145	
304	2.4829	0.00140	0.00001
305	2.4843	0.00140	0
307	2.4871		

Hence Equation (5) gives

$\log_{10} 301 = 2.4771 + 0.00145 + (-3)(-0.00001) = 2.4786$, as before .

It is clear that the arithmetic in this method is much simpler when compared to that in Lagrange's method.

Example 2:

Using the following table find $f(x)$ as a polynomial in x.

x	$f(x)$
-1	3
0	-6
3	39
6	822
7	1611

The divided difference table is

x	$f(x)$				
-1	3	-9	6	5	1
0	-6	15	41	13	
3	39	261	132		
7	822	789			

Hence Equation (5) gives

$$f(x) = 3 + (x+1)(-9) + x(x+1)(6) + x(x+1)(x-3)(5) + x(x+1)(x-3)(x-6)$$
$$= x^4 - 3x^3 + 5x^2 - 6$$

EXERCISES:

1. Prove that (a) $\Delta = \mu\delta + \frac{\delta^2}{2}$

   (b) $\Delta^3 y_2 = \nabla^3 y_5$

2 .From the table of cubes given below, find $(6.36)^3$ and $(6.61)^3$.

x	6.1	6.2	6.3	6.4	6.5	6.6	6.7
x^3	226.981	238.328	250.047	262.144	274.625	287.496	300.763

3. Define the operators $\Delta, \nabla, \delta, E$ and E^{-1} and show that

(a) $\Delta^r y_k = \nabla^r y_{k+r} = \delta^r y_{k+\frac{r}{2}}$

(b) $\Delta\nabla y_k = \nabla\Delta y_k = \delta^2 y_k$

(c) $\mu\delta = \frac{\Delta+\nabla}{2}$

(d) $1 + \mu^2\delta^2 = \left(1 + \frac{1}{2}\delta^2\right)^2$

(e) $\Delta^2 = (1 + \Delta)\delta^2$

(f) $\Delta\left(\frac{1}{y_k}\right) = -\frac{\Delta y_k}{y_k y_{k+1}}$.

4. Show that

$$\left(\Delta - \frac{1}{2}\delta^2\right) = \delta\left(1 + \frac{\delta^2}{4}\right)^{1/2}$$

5.Find the missing terms in the following:

x	0	5	10	15	20	25	30
y	1	3	?	73	225	?	1153

6.Derive expressions for the errors in Newton's formulae of forward and backward differences. Estimate the maximum error made in any value of $\sin x$ in Example 3.6 obtained by interpolation in the range $15° \le x \le 40°$.

7. Certain values of x and $f(x)$ are given below. Find $f(1.235)$.

x	1.00	1.05	1.10	1.15	1.20	1.25
$f(x)$	0.682689	0.706282	0.728668	0.749856	0.769861	0.788700

8. Prove the following relations:

(a) $\delta^2 E = \Delta^2$

(b) $E^{-1/2} = \mu - \frac{\delta}{2}$

(c) $\nabla = \delta E^{-1/2}$

(d) $\Delta - \nabla = \delta^2$

(e) $\mu = \cosh\frac{hD}{2}$.

9. Using Gauss's forward formula, find the value of $f(32)$ given that $f(25) =$

$0.2707, f(30) = 0.3027, f(35) = 0.3386$ and $f(40) = 0.3794$.

10. State Gauss's backward formula and use it to find the value of $\sqrt{12525}$, given that $\sqrt{12500} = 111.8034, \sqrt{12510} = 111.8481$, $\sqrt{12520} = 111.8928, \sqrt{12530} = 111.9375$ and $\sqrt{12540} = 111.9822$.

11.State Stirling's formula for interpolation at the middle of a table of values and find $e^{1.91}$ from the following table:

x	1.7	1.8	1.9	2.0	2.1	2.2
e^x	5.4739	6.0496	6.6859	7.3891	8.1662	9.0250

12. Using Stirling's formula, find $\cos(0.17)$, given that $\cos(0) = 1$, $\cos(0.05) = 0.9988, \cos(0.10) = 0.9950, \cos(0.15) = 0.9888$, $\cos(0.20) = 0.9801, \cos(0.25) = 0.9689$, and $\cos(0.30) = 0.9553$.

13. State Lagrange's interpolation formula and find a bound for the error in linear interpolation.

14. Write an algorithm for Lagrange's formula. Find the polynomial which fits the following data $(-1,7), (1,5)$ and $(2,15)$

15.Find $y(2)$ from the following data using Lagrange's formula

x	0	1	3	4	5
y	0	1	81	256	625

16. Let the values of the function $y = \sin x$ be tabulated at the abscissae $0, \pi/4$ and $\pi/2$. If the Lagrange polynomial $L_2(x)$ is fitted to this data, find a bound for the error in the interpolated value.

17. Establish Newton's divided-difference interpolation formula and give an estimate of the remainder term. Deduce Newton's forward and backward difference interpolation formulae as particular cases.

Unit III

Numerical Differentiation and Integration: Derivatives using Newton's forward difference formula–Derivatives using Newton's backward difference formula – Derivatives using central difference formula – Maxima and Minima of the Interpolating polynomial–Numerical Integration.

Chapter 3: Sections - 3.1 to 3.5

3.1. Introduction:

In Chapter 3, we were concerned with the general problem of interpolation, viz., given the set of values $(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)$ of x and y, to find a polynomial $\phi(x)$ of the lowest degree such that $y(x)$ and $\phi(x)$ agree at the set of tabulated points. In the present chapter, we shall be concerned with the problems of numerical differentiation and integration. That is to say, given the set of values of x and y, as above, we shall derive

formulae to compute:

(i) $\frac{dy}{dx}, \frac{d^2y}{dx^2}, \cdots$ for any value of x in $[x_0, x_n]$, and

(ii) $\int_{x_0}^{x_n} y dx$.

3.2. Numerical Differentiation:

The general method for deriving the numerical differentiation formulae is to differentiate the interpolating polynomial. We illustrate the derivation with Newton's forward difference formula only, the method of derivation being the same with regard to the other formulae.

Consider Newton's forward difference formula:

$$y = y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \cdots, \quad \ldots\ldots\ldots (1)$$

Where $x = x_0 + uh \quad \ldots\ldots\ldots\ldots (2)$

Then $\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx} = \frac{1}{h}\left(\Delta y_0 + \frac{2u-1}{2}\Delta^2 y_0 + \frac{3u^2-6u+2}{6}\Delta^3 y_0 + \cdots\right) \quad \ldots\ldots\ldots\ldots (3)$

This formula can be used for computing the value of dy/dx for non-tabular values of x. For tabular values of x, the formula takes a simpler form, for by setting $x = x_0$ we obtain $u = 0$ from Equation (2), and hence Equation (3) gives

$$\left[\frac{dy}{dx}\right]_{x=x_0} = \frac{1}{h}\left(\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \cdots\right) \quad \ldots\ldots\ldots\ldots (4)$$

Differentiating Equation (3) once again, we obtain

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\left(\Delta^2 y_0 + \frac{6u-6}{6}\Delta^3 y_0 + \frac{12u^2-36u+22}{24}\Delta^4 y_0 + \cdots\right) \quad \ldots\ldots\ldots\ldots (5)$$

from which we obtain $\left[\frac{d^2y}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\left(\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 + \cdots\right)$ ……….. (6)

Formulae for computing higher derivatives may be obtained by successive differentiation. In a similar way, different formulae can be derived by starting with other interpolation formulae. Thus,

(a) Newton's backward difference formula gives

$\left[\frac{dy}{dx}\right]_{x=x_n} = \frac{1}{h}\left(\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \cdots\right)$ …………. (7)

and $\left[\frac{d^2y}{dx^2}\right]_{x=x_n} = \frac{1}{h^2}\left(\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \frac{5}{6}\nabla^5 y_n + \cdots\right)$ ………… (8)

(b) Stirling's formula gives

$\left[\frac{dy}{dx}\right]_{x=x_0} = \frac{1}{h}\left(\frac{\Delta y_{-1} + \Delta y_0}{2} - \frac{1}{6}\frac{\Delta^3 y_{-2} + \Delta^3 y_{-1}}{2} + \frac{1}{30}\frac{\Delta^5 y_{-3} + \Delta^5 y_{-2}}{2} + \cdots\right)$ ………… (9)

and $\left[\frac{d^2y}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\left(\Delta^2 y_{-1} - \frac{1}{12}\Delta^4 y_{-2} + \frac{1}{90}\Delta^6 y_{-3} - \cdots\right)$ ………….. (10)

If a derivative is required near the end of a table, one of the following formulae may be used to obtain better accuracy

$$hy_0' = \left(\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \frac{1}{4}\Delta^4 + \frac{1}{5}\Delta^5 - \frac{1}{6}\Delta^6 + \cdots\right)y_0 \qquad (11)$$

$$= \left(\Delta + \frac{1}{2}\Delta^2 - \frac{1}{6}\Delta^3 + \frac{1}{12}\Delta^4 - \frac{1}{20}\Delta^5 + \frac{1}{30}\Delta^6 - \cdots\right)y_{-1} \qquad (12)$$

$$h^2y_0'' = \left(\Delta^2 - \Delta^3 + \frac{11}{12}\Delta^4 - \frac{5}{6}\Delta^5 + \frac{137}{180}\Delta^6 - \frac{7}{10}\Delta^7 + \frac{363}{560}\Delta^8 - \cdots\right)y_0 \qquad (13)$$

$$= \left(\Delta^2 - \frac{1}{12}\Delta^4 + \frac{1}{12}\Delta^5 - \frac{13}{180}\Delta^6 + \frac{11}{180}\Delta^7 - \frac{29}{560}\Delta^8 + \cdots\right)y_{-1} \qquad (14)$$

$$hy_n' = \left(\nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \frac{1}{4}\nabla^4 + \frac{1}{5}\nabla^5 + \frac{1}{6}\nabla^6 + \frac{1}{7}\nabla^7 + \frac{1}{8}\nabla^8 + \cdots\right)y_n \qquad (15)$$

$$= \left(\nabla - \frac{1}{2}\nabla^2 - \frac{1}{6}\nabla^3 - \frac{1}{12}\nabla^4 - \frac{1}{20}\nabla^5 - \frac{1}{30}\nabla^6 - \frac{1}{42}\nabla^7 - \frac{1}{56}\nabla^8 - \cdots\right)y_{n+1} \qquad (16)$$

$$h^2y_n'' = \qquad (17)$$

$$= \left(\nabla^2 + \nabla^3 + \frac{11}{12}\nabla^4 + \frac{5}{6}\nabla^5 + \frac{137}{180}\nabla^6 + \frac{7}{10}\nabla^7 + \frac{363}{560}\nabla^8 + \cdots\right)y_n \qquad (18)$$

$$= \left(\nabla^2 - \frac{1}{12}\nabla^4 - \frac{1}{12}\nabla^5 - \frac{13}{180}\nabla^6 - \frac{11}{180}\nabla^7 - \frac{29}{560}\nabla^8 - \cdots\right)y_{n+1}. \qquad (19)$$

For more details, the reader is referred to Interpolation and Allied Tables. The following examples illustrate the use of the formulae stated above.

Example 1:

From the following table of values of x and y, obtain dy/dx and d^2y/dx^2 for $x = 1.2$:

x	y	x	y
1.0	2.7183	1.8	6.0496
1.2	3.3201	2.0	7.3891
1.4	4.0552	2.2	9.0250
1.6	4.9530		

The difference table is

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
1.0	2.7183						
		0.6018					
1.2	3.3201		0.1333				
		0.7351		0.0294			
1.4	4.0552		0.1627		0.0067		
		0.8978		0.0361		0.0013	
1.6	4.9530		0.1988		0.0080		0.0001
		1.0966		0.0441		0.0014	
1.8	6.0496		0.2429		0.0094		
		1.3395		0.0535			
2.0	7.3891		0.2964				
		1.6359					
2.2	9.0250						

Here $x_0 = 1.2, y_0 = 3.3201$ and $h = 0.2$. Hence Equation (11) gives

$$\left[\frac{dy}{dx}\right]_{x=1.2} = \frac{1}{0.2}\left[0.7351 - \frac{1}{2}(0.1627) + \frac{1}{3}(0.0361) - \frac{1}{4}(0.0080) + \frac{1}{5}(0.0014)\right]$$
$$= 3.3205$$

If we use formula (12), then we should use the differences diagonally downwards from 0.6018 and this gives

$$\left[\frac{dy}{dx}\right]_{x=1.2} = \frac{1}{0.2}\left[0.6018 + \frac{1}{2}(0.1333) - \frac{1}{6}(0.0294) + \frac{1}{12}(0.0067) - \frac{1}{20}(0.0013)\right]$$
$$= 3.3205, \text{ as before.}$$

Similarly, formula (13) gives

$$\left[\frac{d^2y}{dx^2}\right]_{x=1.2} = \frac{1}{0.04}\left[0.1627 - 0.0361 + \frac{11}{12}(0.0080) - \frac{5}{6}(0.0014)\right] = 3.318$$

Using formula (14), we obtain

$$\left[\frac{d^2y}{dx^2}\right]_{x=1.2} = \frac{1}{0.04}\left[0.1333 - \frac{1}{12}(0.0067) + \frac{1}{12}(0.0013)\right] = 3.32$$

Example 2:

Calculate the first and second derivatives of the function tabulated in the preceding example at the point $x = 2.2$ and also dy/dx at $x = 2.0$.

Solution:

We use the table of differences of Example 1. Here $x_n = 2.2, y_n = 9.0250$ and $h = 0.2$.

Hence formula (15) gives

$$\left[\frac{dy}{dx}\right]_{x=2.2} = \frac{1}{0.2}\left[1.6359 + \frac{1}{2}(0.2964) + \frac{1}{3}(0.0535) + \frac{1}{4}(0.0094) + \frac{1}{5}(0.0014)\right]$$
$$= 9.0228.$$

$$\left[\frac{d^2y}{dx^2}\right]_{x=2.2} = \frac{1}{0.04}\left[0.2964 + 0.0535 + \frac{11}{12}(0.0094) + \frac{5}{6}(0.0014)\right] = 8.992.$$

To find dy/dx at $x = 2.0$, we can use either (6.15) or (6.16). Formula (6.15) gives

$$\left[\frac{dy}{dx}\right]_{x=2.0} = \left.\frac{1}{0.2}\right]\left[1.3395 + \frac{1}{2}(0.2429) + \frac{1}{3}(0.0441) + \frac{1}{4}(0.0080)\right)$$

whereas from formula (6.16), we obtain

$$\left[\frac{dy}{dx}\right]_{x=2.0} = \frac{1}{0.2}\left[1.6359 - \frac{1}{2}(0.2964) - \frac{1}{6}(0.0535) - \frac{1}{12}(0.0094) - \frac{1}{20}(0.0014)\right]$$
$$= 7.3896$$

Example 3:

Find dy/dx and d^2y/dx^2 at $x = 1.6$ for the tabulated function of Example 1.

Choosing $x_0 = 1.6$, formula (9) gives

$$\left[\frac{dy}{dx}\right]_{x=1.6} = \frac{1}{0.2}\left(\frac{0.8978 + 1.0966}{2} - \frac{1}{2}\frac{0.0361 + 0.0441}{2} + \frac{1}{30}\frac{0.0013 + 0.0014}{2}\right)$$
$$= 4.9530$$

Similarly, formula (10) yields

$$\left[\frac{d^2y}{dx^2}\right]_{x=1.6} = \frac{1}{0.04}\left[0.1988 - \frac{1}{12}(0.0080) + \frac{1}{90}(0.0001)\right] = 4.9525$$

In the preceding examples, the tabulated function is e^x and hence it is easy to see that the error is considerably more in the case of the second derivatives. This is due to the reason that although the tabulated function and its approximating polynomial would agree at the set of data points, their slopes at these points may vary considerably. Numerical differentiation, is, therefore, an unsatisfactory process and should be used only in 'rare cases.' The next section will be devoted to a discussion of errors in the numerical differentiation formulae.

3.2.1 Errors in Numerical Differentiation

The numerical computation of derivatives involves two types of errors, viz. truncation errors and rounding errors. These are discussed below.

The truncation error is caused by replacing the tabulated function by means of an interpolating polynomial. This error can usually be estimated by formula (7). As noted earlier, this formula is of theoretical interest only, since, in practical computations, we usually do not have any information about the derivative $y^{(n+1)}(\xi)$. However, the truncation error in any numerical differentiation formula can easily be estimated in the following manner. Suppose that the tabulated function is such that its differences of a certain order are small and that the tabulated function is well approximated by the polynomial. (This means that the tabulated function does not have any rapidly varying components.) We know that 2ε is the total absolute error in the values of $\Delta y_i, 4\varepsilon$ in the values of $\Delta^2 y_i$, etc., where ε is the absolute error in the values of y_i. Consider now, for example, Stirling's formula (9). This can be written in the form

$$\left[\frac{dy}{dx}\right]_{x=x_0} = \frac{\Delta y_{-1}+\Delta y_0}{2h} + T_1 = \frac{y_1 - y_{-1}}{2h} + T_1, \quad \ldots\ldots\ldots\ldots (19)$$

where T_1, the truncation error, is given by

$$T_1 = \frac{1}{6h}\left|\frac{\Delta^3 y_{-2}+\Delta^3 y_{-1}}{2}\right| \quad \ldots\ldots\ldots..(20)$$

Similarly, formula (10) can be written as $\left[\frac{d^2y}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\Delta^2 y_{-1} + T_2$ ....(21)

Where $T_2 = \frac{1}{12h^2}|\Delta^4 y_{-2}|$ ....(22)

The rounding error, on the other hand, is inversely proportional to h in the case of first derivatives, inversely proportional to h^2 in the case of second

derivatives, and so on. Thus, rounding error increases as h decreases. Considering again Stirling's formula in the form of Equation (19), the rounding error does not exceed $2\varepsilon/2h = \varepsilon/h$, where ε is the maximum error in the value of y_i. On the other hand, the formula

$$\left[\frac{dy}{dx}\right]_{x=x_0} = \frac{\Delta y_{-1}+\Delta y_0}{2h} - \frac{\Delta^3 y_{-2}+\Delta^3 y_{-1}}{12h} + \cdots$$

has the maximum rounding error

$$\frac{18\varepsilon}{12h} = \frac{3\varepsilon}{2h}$$

Finally, the formula $\left[\frac{d^2y}{dx^2}\right]_{x=x_0} = \frac{\Delta^2 y_{-1}}{h^2} + \cdots = \frac{y_{-1}-2y_0+y_1}{h^2} + \cdots$ ……..(24)

has the maximum rounding error $4\varepsilon/h^2$. It is clear that in the case of higher derivatives, the rounding error increases rather rapidly.

Example 4:

Assuming that the function values given in the table of Example 1 are correct to the accuracy given, estimate the errors in the values of dy/dx and d^2y/dx^2 at $x = 1.6$.

Since the values are correct to 4D, it follows that $\varepsilon < 0.00005 = 0.5 \times 10^{-4}$.

Value of dy/dx at $x = 1.6$:

$$\text{Truncation error } = \frac{1}{6h}\left|\frac{\Delta^3 y_{-1} + \Delta^3 y_0}{2}\right|, \text{ from equation (20)}$$
$$= \frac{1}{6(0.2)}\frac{0.0361 + 0.0441}{2}$$
$$= 0.03342$$

and

$$\text{Rounding error } = \frac{3\varepsilon}{2h}, \text{ from (23)}$$
$$= \frac{3(0.5)10^{-4}}{0.4}$$
$$= 0.00038$$

Hence,

$$\text{Total error } = 0.03342 + 0.00038 = 0.0338$$

Using Stirling's formula from Equation (19), with the first differences, we obtain

$$\left(\frac{dy}{dx}\right)_{x=1.6} = \frac{\Delta y_{-1} + \Delta y_0}{2h} = \frac{0.8978 + 1.0966}{0.4} = \frac{1.9944}{0.4} = 4.9860.$$

The exact value is 4.9530 so that the error in the above solution is (4.9860 4.9530), i.e., 0.0330, which agrees with the total error obtained above.

Value of d^2y/dx^2 at $x = 1.6$:

Using Equation (24), we obtain

$$\left[\frac{d^2y}{dx^2}\right]_{x=1.6} = \frac{\Delta^2 y_{-1}}{h^2} = \frac{0.1988}{0.04} = 4.9700$$

so that the error $= 4.9700 - 4.9530 = 0.0170$.

Also,

$$\text{Truncation error } = \frac{1}{12h^2}|\Delta^4 y_{-2}| = \frac{1}{12(0.04)} \times 0.0080 = 0.01667$$

and

$$\text{Rounding error } = \frac{4\varepsilon}{h^2} = \frac{4 \times 0.5 \times 10^{-4}}{0.04} = 0.0050$$

Hence

Total error in $\left[\frac{d^2y}{dx^2}\right]_{x=1.6} = 0.0167 + 0.0050 = 0.0217.$

3.2.2. Cubic Spline Method:

The following examples illustrate the use of the spline formulae in numerical differentiation.

Example 5:

We consider the function $y(x) = \sin x$ in $[0, \pi]$.

Here $M_0 = M_N = 0$. Let $N = 2$, i.e., $h = \pi/2$. Then

$y_0 = y_2 = 0, y_1 = 1$ and $M_0 = M_2 = 0$.

Using formulae, we obtain

$$M_0 + 4M_1 + M_2 = \frac{6}{h^2}(y_0 - 2y_1 + y_2)$$

or

$$M_1 = -\frac{12}{\pi^2}$$

Formula now gives the spline in each interval. Thus, in $0 \le x \le \pi/2$, we obtain

$$s(x) = \frac{2}{\pi}\left(\frac{-2x^3}{\pi^2} + \frac{3x}{2}\right)$$

which gives $s'(x) = \frac{2}{\pi}\left[-\frac{2}{\pi^2}(3x^2) + \frac{3}{2}\right]$. ....(i)

Hence

$$s'\left(\frac{\pi}{4}\right) = \frac{2}{\pi}\left(-\frac{6}{\pi^2}\frac{\pi^2}{16} + \frac{3}{2}\right) = \frac{9}{4\pi} = 0.71619725$$

Exact value of $s'(\pi/4) = \cos \pi/4 = 1/\sqrt{2} = 0.70710681$. The percentage error in the computed value of $s'(\pi/4)$ is 1.28%. From (i),

$$s''(x) = -\frac{24}{\pi^3}x$$

and hence

$$s''\left(\frac{\pi}{4}\right) = -\frac{24}{\pi^3}\frac{\pi}{4} = -\frac{6}{\pi^2} = -0.60792710$$

Since the exact value is $-1/\sqrt{2}$, the percentage error in this result is 14.03%. We now consider values of $y = \sin x$ in intervals of $10°$ from $x = 0$ to π. To obtain the spline second derivatives we used a computer and the results are given in the following table (up to $x = 90°$).

	$y''(x)$	
x (in degrees)	Exact	Cubic spline
10	-0.173648178	-0.174089426
20	-0.342020143	-0.342889233
30	-0.500000000	-0.501270524
40	-0.642787610	-0.644420964
50	-0.766044443	-0.767990999
60	-0.866025404	-0.868226016
70	-0.939692621	-0.942080425
80	-0.984807753	-0.987310197
90	-1.000000000	-1.002541048

It is seen that there is greater inaccuracy in the values of the spline second derivatives.

Example 6:

From the following data for $y(x)$, find $y'(1.0)$.

x	-2	-1	2	3
$y(x)$	-12	-8	3	5

The function from which the above data was calculated is given by $y = -\frac{1}{15}x^3 - \frac{3}{20}x^2 + \frac{241}{60}x - 3.9$. Hence, the exact value of $y'(1)$ is 3.51667.

To apply the cubic spline formula (5.31), we observe that $h_1 = 1$, $h_2 = 3$ and $h_3 = 1$.

For $i = 1,2$, the recurrence relation gives:

$8M_1 + 3M_2 = -2$

and

$3M_1 + 8M_2 = -10$

since $M_0 = M_3 = 0$. We obtain $M_1 = \frac{14}{55}$ and $M_2 = -\frac{74}{55}$. In $-1 \leq x \leq 2$, we have

$$s_2(x) = \frac{1}{3}\left[\frac{(2-x)^3}{6}\cdot\frac{14}{55} + \frac{(x+1)^3}{6}\left(-\frac{74}{55}\right)\right]$$
$$+\frac{1}{3}\left[-8-\frac{21}{55}\right](2-x) + \frac{1}{3}\left[3-\frac{9}{6}\left(-\frac{74}{55}\right)\right](x+1)$$

Differentiating the above and putting $x = 1$, we obtain

$$y'(1) \approx s_2'(1.0) = \frac{1}{3}\left[-\frac{7}{55} - \frac{148}{55} + \frac{461}{55} + \frac{276}{55}\right]$$
$$= 3.52727, \text{ on simplification.}$$

3.2.3 Differentiation Formulae with Function Values

In Section 3.2, we developed forward, backward and central difference approximations of derivatives in terms of finite differences. From the computational point of view, it would be convenient to express the numerical differentiation formulae in terms of function values. We list below some differentiation formulae for use in numerical computations.

(i) Forward Differences

$$y'(x_i) = \frac{y_{i+1} - y_i}{h}; \qquad y'(x_i) = \frac{-y_{i+2} + 4y_{i+1} - 3y_i}{2h} + O(h^2)$$
$$y''(x_i) = \frac{y_i - 2y_{i+1} + y_{i+2}}{h^2}; \quad y''(x_i) = \frac{-y_{i+3} + 4y_{i+2} - 5y_{i+1} + 2y_i}{h^2}$$

(ii) Backward Differences

$$y'(x_i) = \frac{y_i - y_{i-1}}{h}; \qquad y'(x_i) = \frac{3y_i - 4y_{i-1} + y_{i-2}}{2h};$$
$$y''(x_i) = \frac{y_i - 2y_{i-1} + y_{i-2}}{h^2}; \quad y''(x_i) = \frac{2y_i - 5y_{i-1} + 4y_{i-2} - y_{i-3}}{h^2};$$

(iii) Central Differences

$$y'(x_i) = \frac{y_{i+1} - y_{i-1}}{2h}; \; y'(x_i) = \frac{-y_{i+2} + 8y_{i+1} - 8y_{i-1} + y_{i-2}}{12h};$$
$$y''(x_i) = \frac{y_{i-1} - 2y_i + y_{i+1}}{h^2};$$
$$y''(x_i) = \frac{-y_{i+2} + 16y_{i+1} - 30y_i + 16y_{i-1} - y_{i-2}}{12h^2}$$

These formulae can be derived by using Taylor series expansion of the functions.

3.3. Maximum and Minimum Values of a Tabulated Function:

It is known that the maximum and minimum values of a function can be found by equating the first derivative to zero and solving for the variable. The same procedure can be applied to determine the maxima and minima of a tabulated function. Consider Newton's forward difference formula

$$y = y_0 + p\Delta y_0 + \frac{p(p-1)}{2}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{6}\Delta^3 y_0 + \cdots$$

Differentiating this with respect to p, we obtain

$$\frac{dy}{dp} = \Delta y_0 + \frac{2p-1}{2}\Delta^2 y_0 + \frac{3p^2-3p+2}{6}\Delta^3 y_0 + \cdots \quad \ldots\ldots\ldots(1)$$

For maxima or minima $dy/dp = 0$. Hence, terminating the right-hand side, for simplicity, after the third difference and equating it to zero, we obtain the quadratic for p

$$c_0 + c_1 p + c_2 p^2 = 0 \ \ldots\ldots\ldots(2)$$

where

$$\left.\begin{aligned} c_0 &= \Delta y_0 - \tfrac{1}{2}\Delta^2 y_0 + \tfrac{1}{3}\Delta^3 y_0 \\ \text{and } c_1 &= \Delta^2 y_0 - \Delta^3 y_0 \\ c_2 &= \tfrac{1}{2}\Delta^3 y_0 \end{aligned}\right\} \quad \ldots\ldots\ldots\ldots(3)$$

Values of x can then be found from the relation $x = x_0 + ph$.

Example 1:

From the following table, find x, correct to two decimal places, for which y is maximum and find this value of y.

x	y
1.2	0.9320
1.3	0.9636
1.4	0.9855

1.5	0.9975
1.6	0.9996

The table of differences is

x	y	Δ	Δ^2
1.2	0.9320		
		0.0316	
1.3	0.9636		−0.0097
		0.0219	
1.4	0.9855		−0.0099
		0.0120	
1.5	0.9975		−0.0099
		0.0021	
1.6	0.9996		

Let $x_0 = 1.2$. Then formula (1), terminated after second differences, gives

$$0 = 0.0316 + \frac{2p-1}{2}(-0.0097)$$

from which we obtain $p = 3.8$. Hence

$$x = x_0 + ph = 1.2 + (3.8)(0.1) = 1.58.$$

For this value of x, Newton's backward difference formula at $x_n = 1.6$ gives

$$\begin{aligned} y(1.58) &= 0.9996 - 0.2(0.0021) + \frac{-0.2(-0.2+1)}{2}(-0.0099) \\ &= 0.9996 - 0.0004 + 0.0008 \\ &= 1.0 \end{aligned}$$

3.4.Numerical Integration:

The general problem of numerical integration may be stated as follows. Given a set of data points $(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n)$ of a function $y = f(x)$, where $f(x)$ is not known explicitly, it is required to compute the value of the definite integral

$$I = \int_a^b y\,dx \quad \ldots\ldots\ldots\ldots(1)$$

As in the case of numerical differentiation, one replaces $f(x)$ by an interpolating polynomial $\phi(x)$ and obtains, on integration, an approximate value of the definite integral. Thus, different integration formulae can be obtained depending upon the type of the interpolation formula used. We derive in this section a general formula for numerical integration using Newton's forward difference formula.

Let the interval $[a, b]$ be divided into n equal subintervals such that

$a = x_0 < x_1 < x_2 < \cdots x_n = b$. Clearly, $x_n = x_0 + nh$. Hence the integral becomes

$$I = \int_{x_0}^{x_n} y dx$$

Approximating y by Newton's forward difference formula, we obtain

$$I = \int_{x_0}^{x_n} \left[y_0 + p\Delta y_0 + \frac{p(p-1)}{2}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{6}\Delta^3 y_0 + \cdots\right] dx$$

Since $x = x_0 + ph, dx = hdp$ and hence the above integral becomes

$$I = h\int_{0}^{n} \left[y_0 + p\Delta y_0 + \frac{p(p-1)}{2}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{6}\Delta^3 y_0 + \cdots\right] dp$$

which gives on simplification

$$\int_{x_0}^{x_n} y dx = nh\left[y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{12}\Delta^2 y_0 + \frac{n(n-2)^2}{24}\Delta^3 y_0 + \cdots\right] \quad \text{..........(2)}$$

From this general formula, we can obtain different integration formulae by putting $n = 1,2,3, \ldots$, etc. We derive here a few of these formulae but it should be remarked that the trapezoidal and Simpson's $1/3$-rules are found to give sufficient accuracy for use in practical problems.

3.4.1.Trapezoidal Rule:

Setting $n = 1$ in the general formula (2), all differences higher than the first will become zero and we obtain

$$\int_{x_0}^{x_1} y dx = h\left(y_0 + \frac{1}{2}\Delta y_0\right) = h\left[y_0 + \frac{1}{2}(y_1 - y_0)\right] = \frac{h}{2}(y_0 + y_1). \quad \text{.....(3)}$$

For the next interval $[x_1, x_2]$, we deduce similarly

$\int_{x_1}^{x_2} ydx = \frac{h}{2}(y_1 + y_2)$ ………. (4)

and so on. For the last interval $[x_{n-1}, x_n]$, we have

$\int_{x_{n-1}}^{x_n} ydx = \frac{h}{2}(y_{n-1} + y_n)$ ………….. (5)

Combining all these expressions, we obtain the rule

$\int_{x_0}^{x_n} ydx = \frac{h}{2}[y_0 + 2(y_1 + y_2 + \cdots + y_{n-1}) + y_n]$ …………(6)

which is known as the trapezoidal rule.

The geometrical significance of this rule is that the curve $y = f(x)$ is replaced by n straight lines joining the points (x_0, y_0) and (x_1, y_1); (x_1, y_1) and (x_2, y_2), … , (x_{n-1}, y_{n-1}) and (x_n, y_n). The area bounded by the curve $y = f(x)$, the ordinates $x = x_0$ and $x = x_n$, and the x-axis is then approximately equivalent to the sum of the areas of the n trapeziums obtained.

The error of the trapezoidal formula can be obtained in the following way. Let $y = f(x)$ be continuous, well-behaved, and possess continuous derivatives in $[x_0, x_n]$. Expanding y in a Taylor's series around $x = x_0$, we obtain

$$\int_{x_0}^{x_1} ydx = \int_{x_0}^{x_1}\left[y_0 + (x - x_0)y_0' + \frac{(x - x_0)^2}{2}y_0'' + \cdots\right]dx$$

$= hy_0 + \frac{h^2}{2}y_0' + \frac{h^3}{6}y_0'' + \cdots$ …. ……….(7)

Similarly,

$$\frac{h}{2}(y_0 + y_1) = \frac{h}{2}\left(y_0 + y_0 + hy_0' + \frac{h^2}{2}y_0'' + \frac{h^3}{6}y_0''' + \cdots\right)$$

$= hy_0 + \frac{h^2}{2}y_0' + \frac{h^3}{4}y_0''' + \cdots$ …. …………..(8)

From Equations. (4) and (5), we obtain

$\int_{x_0}^{x_1} ydx - \frac{h}{2}(y_0 + y_1) = -\frac{1}{12}h^3 y_0'' + \cdots$ …………(9)

which is the error in the interval $[x_0, x_1]$. Proceeding in a similar manner we obtain the errors in the remaining subintervals, viz., $[x_1, x_2], [x_2, x_3], \ldots$ and $[x_{n-1}, x_n]$. We thus have $E = -\frac{1}{12}h^3(y_0'' + y_1'' + \cdots + y_{n-1}'')$ ……….(10)

where E is the total error. Assuming that $y''(\bar{x})$ is the largest value of the n quantities on the right-hand side of Equation (10), we obtain

$$E = -\frac{1}{12}h^3 n y''(\bar{x}) = -\frac{b-a}{12}h^2 y''(\bar{x}) \quad \ldots\ldots\ldots..(11)$$

since $nh = b - a$.

3.4.2. Simpson's 1/3-Rule:

This rule is obtained by putting $n = 2$ in Equation (2), i.e. by replacing the curve by $n/2$ arcs of second-degree polynomials or parabolas. We have then

$$\int_{x_0}^{x_2} y dx = 2h\left(y_0 + \Delta y_0 + \frac{1}{6}\Delta^2 y_0\right) = \frac{h}{3}(y_0 + 4y_1 + y_2).$$

Similarly,

$$\int_{x_2}^{x_4} y dx = \frac{h}{3}(y_2 + 4y_3 + y_4)$$
$$\vdots$$

and finally

$$\int_{x_{n-2}}^{x_n} y dx = \frac{h}{3}(y_{n-2} + 4y_{n-1} + y_n)$$

Summing up, we obtain

$$\int_{x_0}^{x_n} y dx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + y_5 + \cdots + y_{n-1}) + 2(y_2 + y_4 + y_6 + \cdots + y_{n-2}) + y_n]$$

…………..(12)

which is known as Simpson's $1/3$-rule, or simply Simpson's rule. It should be noted that this rule requires the division of the whole range into an even number of subintervals of width h.

Following the method outlined in Section 3.4.1, it can be shown that the error in Simpson's rule is given by

$$\int_a^b ydx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + y_5 + \cdots + y_{n-1})$$
$$+2(y_2 + y_4 + y_6 + \cdots + y_{n-2}) + y_n]$$

$$= \frac{b-a}{180} h^4 y^{\text{iv}}(\bar{x}) \qquad \ldots\ldots\ldots\ldots\ldots(13)$$

where $y^{\text{iv}}(\bar{x})$ is the largest value of the fourth derivatives.

3.4.3 Simpson's 3/8-Rule

Setting $n = 3$ in Equation (2), we observe that all the differences higher than the third will become zero and we obtain

$$\int_{x_0}^{x_3} ydx = 3h\left(y_0 + \frac{3}{2}\Delta y_0 + \frac{3}{4}\Delta^2 y_0 + \frac{1}{8}\Delta^3 y_0\right)$$
$$= 3h\left[y_0 + \frac{3}{2}(y_1 - y_0) + \frac{3}{4}(y_2 - 2y_1 + y_0) + \frac{1}{8}(y_3 - 3y_2 + 3y_1 - y_0)\right]$$
$$= \frac{3h}{8}(y_0 + 3y_1 + 3y_2 + y_3)$$

Similarly

$$\int_{x_3}^{x_6} ydx = \frac{3h}{8}(y_3 + 3y_4 + 3y_5 + y_6)$$

and so on. Summing up all these, we obtain

$$\int_{x_0}^{x_n} ydx = \frac{3h}{8}[(y_0 + 3y_1 + 3y_2 + y_3) + (y_3 + 3y_4 + 3y_5 + y_6) + \cdots$$
$$+ (y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n)$$

$$= \frac{3h}{8}(y_0 + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + \cdots. + 2y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n)$$

$$\ldots\ldots\ldots\ldots(14)$$

This rule, called Simpson's (3/8)-rule, is not so accurate as Simpson's rule, the dominant term in the error of this formula being $-(3/80)h^5 y^{\text{iv}}(\bar{x})$.

3.4.4. Boole's and Weddle's Rules:

If we wish to retain differences up to those of the fourth order, we should integrate between x_0 and x_4 and obtain Boole's formula

$$\int_{x_0}^{x_4} y dx = \frac{2h}{45}(7y_0 + 32y_1 + 12y_2 + 32y_3 + 7y_4) \quad \ldots\ldots\ldots\ldots(15)$$

The leading term in the error of this formula can be shown to be

$$-\frac{8h^7}{945} y^{\text{vi}}(\bar{x})$$

If, on the other hand, we integrate between x_0 and x_6 retaining differences up to those of the sixth order, we obtain Weddle's rule

$$\int_{x_0}^{x_6} y dx = \frac{3h}{10}(y_0 + 5y_1 + y_2 + 6y_3 + y_4 + 5y_5 + y_6) \quad \ldots\ldots\ldots\ldots(16)$$

the error in which is given by $-(h^7/140)y^{\text{vi}}(\bar{x})$.

These two formulae can also be generalized as in the previous cases. It should, however, be noted that the number of strips will have to be a multiple of four in the case of Boole's rule and a multiple of six for Weddle's rule.

3.4.5. Use of Cubic Splines:

If $s(x)$ is the cubic spline in the interval (x_{i-1}, x_i), then we have

$$I = \int_{x_0}^{x_n} y dx \approx$$

$$= \sum_{i=1}^{n} \int_{x_{i-1}}^{n} \int_{x_{i-1}}^{x_i} s(x) dx$$

$$\left\{ \frac{1}{6h} [(x_i - x)^3 M_{i-1} + (x - x_{i-1})^3 M_i] \right.$$

$$\left. + \frac{1}{h}(x_i - x)\left(y_{i-1} - \frac{h^2}{6} M_{i-1}\right) + \frac{1}{h}(x - x_{i-1})\left(y_i - \frac{h^2}{6} M_i\right) \right\} dx$$

On carrying out the integration and simplifying, we obtain

$$I = \sum_{i=1}^{n} \left[\frac{h}{2}(y_{i-1} + y_i) - \frac{h^3}{24}(M_{i-1} + M_i)\right] \ldots\ldots\ldots(17)$$

where M_i, the spline second-derivatives, are calculated from the recurrence relation

$$M_{i-1} + 4M_i + M_{i+1} = \frac{6}{h^2}(y_{i-1} - 2y_i + y_{i+1}), i = 1,2, \ldots, n - 1$$

3.4.6. Romberg Integration:

This method can often be used to improve the approximate results obtained by the finite-difference methods. Its application to the numerical evaluation of definite integrals, for example in the use of trapezoidal rule, can be described, as follows. We consider the definite integral

$$I = \int_a^b y dx$$

and evaluate it by the trapezoidal rule equation (6) with two different subintervals of widths h_1 and h_2 to obtain the approximate values I_1 and I_2, respectively. Then Eq. (6.38) gives the errors E_1 and E_2 as

$$E_1 = -\frac{1}{12}(b - a)h_1^2 y''(\bar{x}) \quad \ldots\ldots\ldots\ldots(18)$$

and $E_2 = -\frac{1}{12}(b - a)h_2^2 y''(\bar{\bar{x}})$ …………(19)

Since the term $y''(\bar{\bar{x}})$ in Eq. (6.46) is also the largest value of $y''(x)$, it is reasonable to assume that the quantities $y''(\bar{x})$ and $y''(\bar{\bar{x}})$ are very nearly the same. We therefore have

$$\frac{E_1}{E_2} = \frac{h_1^2}{h_2^2}$$

and hence

$$\frac{E_2}{E_2 - E_1} = \frac{h_2^2}{h_2^2 - h_1^2}$$

Since $E_2 - E_1 = I_2 - I_1$, this gives $E_2 = \frac{h_2^2}{h_2^2 - h_1^2}(I_2 - I_1)$ ……….(20)

We therefore obtain a new approximation I_3 defined by $I_3 = I_2 - E_2 = \frac{I_1 h_2^2 - I_2 h_1^2}{h_2^2 - h_1^2}$ …..(21)

which, in general, would be closer to the actual value-provided that the errors decrease monotonically and are of the same sign.

If we now set

$$h_2 = \frac{1}{2} h_1 = \frac{1}{2} h$$

Equation (6.48) can be written in the more convenient form

$$I\left(h, \frac{1}{2}h\right) = \frac{1}{3}\left[4I\left(\frac{1}{2}h\right) - I(h)\right] \qquad \ldots\ldots\ldots\ldots(22)$$

where $I(h) = I_1$,

$$I\left(\frac{1}{2}h\right) = I_2 \text{ and } I\left(h, \frac{1}{2}h\right) = I_3.$$

With this notation the following table can be formed

$I(h)$			
	$I\left(h, \frac{1}{2}h\right)$		
		$I\left(h, \frac{1}{2}h, \frac{1}{4}h\right)$	
$I\left(\frac{1}{2}h\right)$			$I\left(h, \frac{1}{2}h, \frac{1}{4}h, \frac{1}{8}h\right)$
	$I\left(\frac{1}{2}h, \frac{1}{4}h\right)$		
$I\left(\frac{1}{4}h\right)$		$I\left(\frac{1}{2}h, \frac{1}{4}h, \frac{1}{8}h\right)$	
	$I\left(\frac{1}{4}h, \frac{1}{8}h\right)$		
$I\left(\frac{1}{8}h\right)$			

The computations can be stopped when two successive values are sufficiently close to each other. This method, due to L.F. Richardson, is called the deferred approach to the limit and the systematic tabulation of this is called Romberg Integration.

3.4.7 Newton-Cotes Integration Formulae:

Let the interpolation points, x_i, be equally spaced, i.e. let $x_i = x_0 + ih$, $i = 0,1,2,\dots,n$, and let the end points of the interval of integration be placed such that

$$x_0 = a. x_n = b, h = \frac{b-a}{n}.$$

Then the definite integral $I = \int_a^b ydx$ ....(23)

is evaluated by an integration formula of the type $I_n = \sum_{i=0}^{n} C_i y_i$ ....(24)

where the coefficients C_i are determined completely by the abscissae x_i. Integration formulae of the type (24) are called Newton-Cotes closed integration formulae. They are 'closed' since the end points a and b are the extreme abscissae in the formulae. It is easily seen that the integration formulae derived in Equations. (21)-(24) are the simplest Newton-Cotes closed formulae.

On the other hand, formulae which do not employ the end points are called Newton-Cotes, open integration formulae. We give below the five simplest Newton-Cotes open integration formulae

(a) $\int_{x_0}^{x_2} ydx = 2hy_1 + \frac{h^3}{3} y''(\bar{x}), (x_0 < \bar{x} < x_2)$ ....(25)

(b) $\int_{x_0}^{x_3} ydx = \frac{3h}{2}(y_1 + y_2) + \frac{3h^3}{4} y''(\bar{x}), (x_0 < \bar{x} < x_3)$ ....(26)

(c) $\int_{x_0}^{x_4} ydx = \frac{4h}{3}(2y_1 - y_2 + 2y_3) + \frac{14}{45} h^5 y^{\text{iv}}(\bar{x}), (x_0 < \bar{x} < x_4)$ ....(27)

(d) $\int_{x_0}^{x_5} ydx = \frac{5h}{24}(11y_1 + y_2 + y_3 + 11y_4) + \frac{95}{144} h^5 y^{\text{iv}}(\bar{x}), (x_0 < \bar{x} < x_5)$ ....(28)

(e) $\int_{x_0}^{x_6} ydx = \frac{6h}{20}(11y_1 - 14y_2 + 26y_3 - 14y_4 + 11y_5) + \frac{41}{140} h^7 y^{\text{vi}}(\bar{x})$, ...(29)

$(x_0 < \bar{x} < x_6)$

A convenient method for determining the coefficients in the Newton-Cotes formulae is the method of undetermined coefficients.

Example 1:

Find, from the following table, the area bounded by the curve and the x-axis from

$x = 7.47$ to $x = 7.52$

x	$f(x)$	x	$f(x)$
7.47	1.93	7.50	2.01
7.48	1.95	7.51	2.03
7.49	1.98	7.52	2.06

We know that

$$\text{Area} = \int_{7.47}^{7.52} f(x)dx$$

with $h = 0.01$, the trapezoidal rule given in Equation(6) of 3.4.1 gives

$$\text{Area} = \frac{0.01}{2}[1.93 + 2(1.95 + 1.98 + 2.01 + 2.03) + 2.06] = 0.0996.$$

Example 2:

A solid of revolution is formed by rotating about the x-axis the area between the x-axis, the lines $x = 0$ and $x = 1$, and a curve through the points with the following coordinates:

x	y
0.00	1.0000
0.25	0.9896
0.50	0.9589
0.75	0.9089
1.00	0.8415

Estimate the volume of the solid formed, giving the answer to three decimal places.

If V is the volume of the solid formed, then we know that

$$V = \pi \int_0^1 y^2 dx$$

Hence we need the values of y^2 and these are tabulated below, correct to four decimal places

x	y^2

0.00	1.0000
0.25	0.9793
0.50	0.9195
0.75	0.8261
1.00	0.7081

With $h = 0.25$, Simpson's rule gives

$$V = \frac{\pi(0.25)}{3}[1.0000 + 4(0.9793 + 0.8261) + 2(0.9195) + 0.7081]$$
$$= 2.8192$$

Example 3:

Evaluate $I = \int_0^1 \frac{1}{1+x} dx$

correct to three decimal places.

We solve this example by both the trapezoidal and Simpson's rules with $h = 0.5, 0.25$ and 0.125 respectively.

(i) $h = 0.5$: The values of x and y are tabulated below:

x	y
0.0	1.0000
0.5	0.6667
1.0	0.5000

(a) Trapezoidal rule gives

$$I = \frac{1}{4}[1.0000 + 2(0.6667) + 0.5] = 0.70835$$

(b) Simpson's rule gives

$$I = \frac{1}{6}[1.0000 + 4(0.6667) + 0.5] = 0.6945$$

(ii) $h = 0.25$: The tabulated values of x and y are given below:

x	y

0.00	1.0000
0.25	0.8000
0.50	0.6667
0.75	0.5714
1.00	0.5000

(a) Trapezoidal rule gives

$$I = \frac{1}{8}[1.0 + 2(0.8000 + 0.6667 + 0.5714) + 0.5] = 0.6970.$$

(b) Simpson's rule gives

$$I = \frac{1}{12}[1.0 + 4(0.8000 + 0.5714) + 2(0.6667) + 0.5] = 0.6932$$

(iii) Finally, we take $h = 0.125$: The tabulated values of x and y are

x	y	x	y
0	1.0	0.625	0.6154
0.125	0.8889	0.750	0.5714
0.250	0.8000	0.875	0.5333
0.375	0.7273	1.0	0.5
0.5	0.6667		

(a) Trapezoidal rule gives

$$I = \frac{1}{16}[1.0 + 2(0.8889 + 0.8000 + 0.7273 + 0.6667) + 0.6154 + 0.5714 + 0.5333) + 0.5]$$
$$= 0.6941$$

(b) Simpson's rule gives

$$I = \frac{1}{24}[1.0 + 4(0.8889 + 0.7273 + 0.6154 + 0.5333)$$
$$+2(0.8000 + 0.6667 + 0.5714) + 0.5]$$
$$=0.6932$$

Hence the value of I may be taken to be equal to 0.693 , correct to three decimal places. The exact value of I is $\log_e 2$, which is equal to 0.693147 .... This example demonstrates that, in general, Simpson's rule yields more accurate results than the trapezoidal rule.

Example 4:

Use Romberg's method to compute $I = \int_0^1 \frac{1}{1+x} dx$

correct to three decimal places.

We take $h = 0.5, 0.25$ and 0.125 successively and use the results obtained in the previous example. We therefore have

$$I(h) = 0.7084, I\left(\frac{1}{2}h\right) = 0.6970, \text{ and } I\left(\frac{1}{4}h\right) = 0.6941$$

Hence, using Eq. (6.49), we obtain

$$I\left(h, \frac{1}{2}h\right) = 0.6970 + \frac{1}{3}(0.6970 - 0.7084) = 0.6932.$$

$$I\left(\frac{1}{2}h, \frac{1}{4}h\right) = 0.6941 + \frac{1}{3}(0.6941 - 0.6970) = 0.6931$$

Finally,

$$I\left(h, \frac{1}{2}h, \frac{1}{4}h\right) = 0.6931 + \frac{1}{3}(0.6931 - 0.6932) = 0.6931$$

The table of values is, therefore,

0.7084		
	0.6932	
0.6970		0.6931
	0.6931	
0.6941		

An obvious advantage of this method is that the accuracy of the computed value is known at each step.

Example 5:

Apply trapezoidal and Simpson's rules to the integral

$$I = \int_0^1 \sqrt{1 - x^2} dx$$

continually halving the interval h for better accuracy.

Using $10,20,30,40$ and 50 subintervals successively, an electronic computer, with a nine decimal precision, produced the results given in Table below. The true value of the integral is $\pi/4 = 0.785398163$.

No. of subintervals	Trapezoidal rule	Simpson's rule
10	0.776129582	0.781752040
20	0.782116220	0.784111766
30	0.783610789	0.784698434
40	0.784236934	0.784943838
50	0.784567128	0.785073144

Example 6:

Evaluate $I = \int_0^1 \sin \pi x dx$

using the cubic spline method.

The exact value of I is $2/\pi = 0.63661978$. To make the calculations easier, we take $n = 2$, i.e. $h = 0.5$. In this case, the table of values of x and $y = \sin px$ is

x	y
0	0
0.5	1.0
1.0	0.0

with $M_0 = M_2 = 0$, we obtain $M_1 = -12$. Then formula equation (17) of 3.4.5 gives

$$I = \frac{1}{4}(y_0 + y_1) - \frac{1}{192}(M_0 + M_1) + \frac{1}{4}(y_1 + y_2) - \frac{1}{192}(M_1 + M_2)$$
$$= \frac{1}{4} + \frac{1}{16} + \frac{1}{4} + \frac{1}{16}$$
$$= \frac{5}{8}$$
$$= 0.62500000$$

which shows that the absolute error in the natural spline solution is 0.01161978 . It is easily verified that the Simpson's rule gives a value with an absolute error 0.03004689 , which is more than the error in the spline solution.

Example 7:

Derive Simpson's 1/3-rule using the method of undetermined coefficients.

We assume the formula

$$\int_{-h}^{h} ydx = a_{-1}y_{-1} + a_0y_0 + a_1y_1 \qquad (i)$$

where the coefficients a_{-1}, a_0 and a_1 have to be determined. For this, we assume that formula (i) is exact when $y(x)$ is $1, x$ or x^2. Putting, therefore, $y(x) = 1, x$ and x^2 successively in (i), we obtain the relations

and

$$a_{-1} + a_0 + a_1 = \int_{-h}^{h} dx = 2h, \qquad (ii)$$

$$-a_{-1} + a_1 = \int_{-h}^{h} xdx = 0 \qquad (iii)$$

$$a_{-1} + a_1 = \frac{2}{3}h \qquad (iv)$$

Solving (ii), (iii) and (iv) for a_{-1}, a_0 and a_1, we obtain

$$a_{-1} = \frac{2}{3} = a_1 \text{ and } a_0 = \frac{4h}{3}.$$

Exercises:

1.Find $\frac{d}{dx}J_0(x)$ at x=0.1 from the following table:

(0, 1.0) ,(0.1,0.9975), (0.2, 0.9900), (0.3, 0.9776), (0.4,0.9604).

2. Tabulate the function $y = f(x) = x^3 - 10x + 6$ at $x_0 = -0.5, x_1 = 1.00$ and $x_2 = 2.0$. Compute its first and second derivatives at x=1.00 using Lagrange's interpolation formula. Compare your results with true values.

3. From the following values of x and y, find $\frac{dy}{dx}$ at x=2 using the cubic spine method.

(2,11) (3,49) (4,123)

4. Evaluate (a) $\int_0^{\pi} x\, sinx\, dx$ (b)$\int_{-2}^{2} \frac{x}{5+2x}\, dx$

using the trapezoidal rule with five ordinates.

5. Using Simpson's $\frac{1}{3}$ – rule with h=1, evaluate the integral I=$\int_3^7 x^2\, logx\, dx$.

Unit IV

Numerical Solutions of Ordinary Differential Equations: Taylor's Series Method – Picard's method – Euler's method – Runge - Kutta method.

Chapter 4: Sections - 4.1 to 4.4

4.1 Introduction:

Many problems in science and engineering can be reduced to the problem of solving differential equations satisfying certain given conditions. The analytical methods of solution, with which the reader is assumed to be familiar, can be applied to solve only a selected class of differential equations. Those equations which govern physical systems do not possess, in general closed form solutions, and hence recourse must be made to numerical methods for solving such differential equations.

To describe various numerical methods for the solution of ordinary differential equations, we consider the general first order differential equation $\frac{dy}{dx} = f(x, y)$ ………..(1)

with the initial condition, $y(x_0) = y_0$ ……….(2)

and illustrate the theory with respect to this equation. The methods so developed can, in general, be applied to the solution of systems of first-order equations, and will yield the solution in one of the two forms:

(i) A series for y in terms of powers of x, from which the value of y can be obtained by direct substitution.

(ii) A set of tabulated values of x and y.

The methods of Taylor and Picard belong to class (i), whereas those of Euler, Runge-Kutta, Adams-Bashforth, etc., belong to class (ii). These latter methods are called step-by-step methods or marching methods because the values of y are computed by short steps ahead for equal intervals h of the independent variable. In the methods of Euler and Runge-Kutta, the interval length h should be kept small and hence these methods can be applied for tabulating y over a limited range only. If, however, the function values are desired over a wider range, the methods due to Adams-Bashforth, AdamsMoulton, Milne, etc., may be used. These methods use finite-differences and require 'starting values' which are usually obtained by Taylor's series or Runge-Kutta methods.

It is well-known that a differential equation of the nth order will have n arbitrary constants in its general solution. In order to compute the numerical solution of such an equation, we therefore need n conditions. Problems in which all the initial conditions are specified at the initial point only are called initial value problems. For example, the problem defined by Eqs. (1) is an initial value problem. On the other hand, in problems involving second-and higher-order differential equations, we may prescribe the conditions at two or more points. Such problems are called boundary value problems.

We shall first describe methods for solving initial value problems of the type (8.1), and at the end of the chapter we will outline methods for solving boundary value problems for second-order differential equations.

4.2 Solution by Taylor's Series:

We consider the differential equation $y' = f(x, y)$ .... (1)

with the initial condition $y(x_0) = y_0$ .... (2)

If $y(x)$ is the exact solution of Eq. (1), then the Taylor's series for $y(x)$ around $x = x_0$ is given by $y(x) = y_0 + (x - x_0)y_0' + \frac{(x-x_0)^2}{2!}y_0'' + \cdots$ .... (3)

If the values of y_0', y_0'', ... are known, then Equation (3) gives a power series for y. Using the formula for total derivatives, we can write

$$y'' = f' = f_x + y' f_y = f_x + f f_y$$

where the suffixes denote partial derivatives with respect to the variable concerned. Similarly, we obtain

$$\begin{aligned} y''' = f'' &= f_{xx} + f_{xy} f + f\left(f_{yx} + f_{yy} f\right) + f_y\left(f_x + f_y f\right) \\ &= f_{xx} + 2f f_{xy} + f^2 f_{yy} + f_x f_y + f f_y^2 \end{aligned}$$

and other higher derivatives of y. The method can easily be extended to simultaneous and higher-order differential equations.

Example 1:

From the Taylor series for $y(x)$, find $y(0.1)$ correct to four decimal places if $y(x)$ satisfies $y' = x - y^2$ and $y(0) = 1$

The Taylor series for $y(x)$ is given by

$$y(x) = 1 + xy_0' + \frac{x^2}{2}y_0'' + \frac{x^3}{6}y_0''' + \frac{x^4}{24}y_0^{\text{iv}} + \frac{x^5}{120}y_0^{\text{v}} + \cdots$$

The derivatives y_0', y_0'', ... etc. are obtained thus:

$y'(x) = x - y^2 \qquad y'_0 = -1$

$y''(x) = 1 - 2yy' \qquad y''_0 = 3$

$y'''(x) = -2yy'' - 2y'^2 \qquad y'''_0 = -8$

$y^{\text{iv}}(x) = -2yy''' - 6y'y'' \qquad y^{\text{iv}}_0 = 34$

$y^{\text{v}}(x) = -2yy^{\text{iv}} - 8y'y''' - 6y''^2 \qquad y^{\text{v}}_0 = -186$

Using these values, the Taylor series becomes

$$y(x) = 1 - x + \frac{3}{2}x^2 - \frac{4}{3}x^3 + \frac{17}{12}x^4 - \frac{31}{20}x^5 + \cdots$$

To obtain the value of $y(0.1)$ correct to four decimal places, it is found that the terms up to x^4 should be considered, and we have $y(0.1) = 0.9138$.

Suppose that we wish to find the range of values of x for which the above series, truncated after the term containing x^4, can be used to compute the values of y correct to four decimal places. We need only to write

$$\frac{31}{20}x^5 \leq 0.00005 \text{ or } x \leq 0.126$$

Example 2:

Given the differential equation $y'' - xy' - y = 0$

with the conditions $y(0) = 1$ and $y'(0) = 0$, use Taylor's series method to determine the value of $y(0.1)$.

We have $y(x) = 1$ and $y'(x) = 0$ when $x = 0$. The given differential equation is

$$y''(x) = xy'(x) + y(x) \qquad (i)$$

Hence $y''(0) = y(0) = 1$. Successive differentiation of (i) gives

$$y'''(x) = xy''(x) + y'(x) + y'(x) = xy''(x) + 2y'(x), \qquad (ii)$$

$$y^{\text{iv}}(x) = xy'''(x) + y''(x) + 2y''(x) = xy'''(x) + 3y''(x), \qquad (iii)$$

$$y^{\text{v}}(x) = xy^{\text{iv}}(x) + y'''(x) + 3y'''(x) = xy^{\text{iv}}(x) + 4y'''(x), \qquad (iv)$$

$$y^{\text{vi}}(x) = xy^{\text{v}}(x) + y^{\text{iv}}(x) + 4y^{\text{iv}}(x) = xy^{\text{v}}(x) + 5y^{\text{iv}}(x), \qquad (v)$$

and similarly for higher derivatives. Putting $x = 0$ in (ii) to (v), we obtain

$y'''(0) = 2y'(0) = 0, y^{\text{iv}}(0) = 3y''(0) = 3, y^{\text{v}}(0) = 0, y^{\text{vi}}(0) = 5.$

By Taylor's series, we have

$$y(x) = y(0) + xy'(0) + \frac{x^2}{2}y''(0) + \frac{x^3}{6}y'''(0) + \frac{x^4}{24}y^{\text{iv}}(0) + \frac{x^5}{120}y^{\text{v}}(0) + \frac{x^6}{720}y^{\text{vi}}(0) + \cdots$$

Hence

$$y(0.1) = 1 + \frac{(0.1)^2}{2} + \frac{(0.1)^4}{24}(3) + \frac{(0.1)^6}{720}(5) + \cdots$$

$= 1 + 0.005 + 0.0000125$, neglecting the last term

$= 1.0050125$, correct to seven decimal places.

4.3 Picard's Method of Successive Approximations

Integrating the differential equation $y = y_0 + \int_{x_0}^{x} f(x,y)dx$ ……… (1)

Equation (1), in which the unknown function y appears under the integral sign, is called an integral equation. Such an equation can be solved by the method of successive approximations in which the first approximation to y is obtained by putting y_0 for y on right side of Equation (1), and we write

$$y^{(1)} = y_0 + \int_{x_0}^{x} f(x, y_0)dx$$

The integral on the right can now be solved and the resulting $y^{(1)}$ is substituted for y in the integrand of Eq. (1) to obtain the second approximation $y^{(2)}$:

$$y^{(2)} = y_0 + \int_{x_0}^{x} f\left(x, y^{(1)}\right)dx$$

Proceeding in this way, we obtain $y^{(3)}, y^{(4)}, \ldots, y^{(n-1)}$ and $y^{(n)}$, where

$$y^{(n)} = y_0 + \int_{x_0}^{x} f\left(x, y^{(n-1)}\right)dx \text{ with } y^{(0)} = y_0 \ldots\ldots\ldots (2)$$

Hence this method yields a sequence of approximations $y^{(1)}, y^{(2)}, \ldots, y^{(n)}$ and it can be proved (see, for example, the book by Levy and Baggot) that if the function $f(x,y)$ is bounded in some region about the point (x_0, y_0) and if $f(x,y)$ satisfies the Lipschitz condition, viz.,

$$|f(x,y) - f(x,\bar{y})| \le K|y - \bar{y}| K \text{ being a constant } \ldots\ldots..(3)$$

then the sequence $y^{(1)}, y^{(2)}, \ldots$ converges to the solution of Eq. (1) of 4.2.

Example 1:

Solve the equation $y' = x + y^2$, subject to the condition $y = 1$ when $x = 0$.

We start with $y^{(0)} = 1$ and obtain

$$y^{(1)} = 1 + \int_{0}^{x} (x+1)dx = 1 + x + \frac{1}{2}x^2$$

Then the second approximation is

$$y^{(2)} = 1 + \int_0^x \left[x + \left(1 + x + \frac{1}{2}x^2\right)^2\right] dx$$
$$= 1 + x + \frac{3}{2}x^2 + \frac{2}{3}x^3 + \frac{1}{4}x^4 + \frac{1}{20}x^5$$

It is obvious that the integrations might become more and more difficult as we proceed to higher approximations.

Example 2:

Given the differential equation $\frac{dy}{dx} = \frac{x^2}{y^2+1}$

with the initial condition $y = 0$ when $x = 0$, use Picard's method to obtain y for $x = 0.25, 0.5$ and 1.0 correct to three decimal places.

We have

$$y = \int_0^x \frac{x^2}{y^2 + 1} dx$$

Setting $y^{(0)} = 0$, we obtain

$$y^{(1)} = \int_0^x x^2 dx = \frac{1}{3}x^3$$

and

$$y^{(2)} = \int_0^x \frac{x^2}{(1/9)x^6 + 1} dx = \tan^{-1}\left(\frac{1}{3}x^3\right) = \frac{1}{3}x^3 - \frac{1}{81}x^9 + \cdots$$

so that $y^{(1)}$ and $y^{(2)}$ agree to the first term, viz., $(1/3)x^3$. To find the range of values of x so that the series with the term $(1/3)x^3$ alone will give the result correct to three decimal places, we put

$$\frac{1}{81}x^9 \leq 0.0005$$

which yields

$$x \leq 0.7$$

Hence

$$y(0.25) = \frac{1}{3}(0.25)^3 = 0.005$$
$$y(0.5) = \frac{1}{3}(0.5)^3 = 0.042$$
$$y(1.0) = \frac{1}{3} - \frac{1}{81} = 0.321$$

4.4 Euler's Method:

We have so far discussed the methods which yield the solution of a differential equation in the form of a power series. We will now describe the methods which give the solution in the form of a set of tabulated values.

Suppose that we wish to solve the Equations. (1) of 4.2 for values of y at $x = x_r = x_0 + rh(r = 1,2, \dots)$. Integrating Eq. (1) of 4.2, we obtain

$y_1 = y_0 + \int_{x_0}^{x_1} f(x,y)dx$ ....(1)

Assuming that $f(x,y) = f(x_0,y_0)$ in $x_0 \le x \le x_1$, this gives Euler's formula

$$y_1 \approx y_0 + hf(x_0,y_0). \dots \dots \dots (1a)$$

Similarly for the range $x_1 \le x \le x_2$, we have

$$y_2 = y_1 + \int_{x_1}^{x_2} f(x,y)dx$$

Substituting $f(x_1,y_1)$ for $f(x,y)$ in $x_1 \le x \le x_2$ we obtain

$$y_2 \approx y_1 + hf(x_1,y_1). \dots \dots . (1b)$$

Proceeding in this way, we obtain the general formula

$$y_{n+1} = y_n + hf(x_n,y_n), n = 0,1,2, \dots \quad \dots \dots \dots (2)$$

The process is very slow and to obtain reasonable accuracy with Euler's method, we need to take a smaller value for h. Because of this restriction

on h, the method is unsuitable for practical use and a modification of it, known as the modified Euler method, which gives more accurate results, will be described in Section 3.4.2.

Example 1:

To illustrate Euler's method, we consider the differential equation $y' = -y$ with the condition $y(0) = 1$.

Successive application of Equation (2) with $h = 0.01$ gives

$$y(0.01) = 1 + 0.1(-1) = 0.99$$
$$y(0.02) = 0.99 + 0.01(-0.99) = 0.9801$$
$$y(0.03) = 0.9801 + 0.01(-0.9801) = 0.9703$$
$$y(0.04) = 0.9703 + 0.01(-0.9703) = 0.9606$$

The exact solution is $y = e^{-x}$ and from this the value at $x = 0.04$ is 0.9608 .

4.4.1 Error Estimates for the Euler Method:

Let the true solution of the differential equation at $x = x_n$ be $y(x_n)$ and also let the approximate solution be y_n. Now, expanding $y(x_{n+1})$ by Taylor's series, we get

$$y(x_{n+1}) = y(x_n) + hy'(x_n) + \frac{h^2}{2}y''(x_n) + \cdots$$

$y(x_{n+1}) = y(x_n) + hy'(x_n) + \frac{h^2}{2}y''(\tau_n) + \cdots$ where $x_n \le \tau_n \le x_{n+1}$ ………..(3)

We usually encounter two types of errors in the solution of differential equations. These are (i) local errors, and (ii) rounding errors. The local error is the result of replacing the given differential equation by means of the equation

$$y_{n+1} = y_n + hy'_n$$

This error is given by $L_{n+1} = -\frac{1}{2}h^2y''(\tau_n)$ ……….(4)

The total error is then defined by $e_n = y_n - y(x_n)$ ………..(5)

Since y_0 is exact, it follows that $e_0 = 0$.

Neglecting the rounding error, we write the total solution error as

$$\begin{aligned} e_{n+1} &= y_{n+1} - y(x_{n+1}) \\ &= y_n + hy'_n - [y(x_n) + hy'(x_n) - L_{n+1}] \\ &= e_n + h[f(x_n, y_n) - y'(x_n)] + L_{n+1}. \end{aligned}$$

$$\Rightarrow\ e_{n+1} = e_n + h\big[f(x_n, y_n) - f\big(x_n, y(x_n)\big)\big] + L_{n+1}.$$

By mean value theorem, we write

$$f(x_n, y_n) - f\big(x_n, y(x_n)\big) = [y_n - y(x_n)]\frac{\partial f}{\partial y}(x_n, \xi_n), y(x_n) \le \xi_n \le y_n$$

Hence, we have

$$e_{n+1} = e_n\big[1 + hf_y(x_n, \xi_n)\big] + L_{n+1} \ \ldots\ldots\ldots (6)$$

Since $e_0 = 0$, we obtain successively:

$$e_1 = L_1;\ e_2 = \big[1 + hf_y(x_1, \xi_1)\big]L_1 + L_2;$$

$$e_3 = \big[1 + hf_y(x_2, \xi_2)\big]\big[1 + hf_y(x_1, \xi_1)\big](L_1 + L_2) + L_3;\ \text{etc.}$$

See the book by Isaacson and Keller [1966] for more details.

Example 2:

We consider, again, the differential equation $y' = -y$ with the condition $y(0) = 1$, which we have solved by Euler's method in Example 1.

Choosing $h = 0.01$, we have

$$1 + hf_y(x_n, \xi_n) = 1 + 0.01(-1) = 0.99$$

and

$$L_{n+1} = -\frac{1}{2}h^2y''(\rho_n) = -0.00005y(\rho_n)$$

In this problem, $y(\rho_n) \leq y(x_n)$, since y' is negative. Hence we successively obtain

$$|L_1| \leq 0.00005 = 5 \times 10^{-5}$$
$$|L_2| \leq (0.00005)(0.99) < 5 \times 10^{-5}$$
$$|L_3| \leq (0.00005)(0.9801) < 5 \times 10^{-5}$$

and so on. For computing the total solution error, we need an estimate of the rounding error. If we neglect the rounding error, i.e., if we set

$R_{n+1} = 0$

then using the above bounds, we obtain from Eq. (8.12) the estimates

$$e_0 = 0$$
$$|e_1| \leq 5 \times 10^{-5}$$
$$|e_2| \leq 0.99e_1 + 5 \times 10^{-5} < 10^{-4}$$
$$|e_3| \leq 0.99e_2 + 5 \times 10^{-5} < 10^{-4} + 5 \times 10^{-5}$$
$$|e_4| \leq 0.99e_3 + 5 \times 10^{-5} < 10^{-4} + 10^{-4} = 2 \times 10^{-4} = 0.0002$$

It can be verified that the estimate for e_4 agrees with the actual error in the value of $y(0.04)$ obtained in Example 1.

4.4.2 Modified Euler's Method:

Instead of approximating $f(x, y)$ by $f(x_0, y_0)$ in Equation (1) of 4.4, we now approximate the integral given in Eq. (8.6) by means of trapezoidal rule to obtain

$$y_1 = y_0 + \frac{h}{2}[f(x_0, y_0) + f(x_1, y_1)] \quad (7)$$

We thus obtain the iteration formula

$$y_1^{(n+1)} = y_0 + \frac{h}{2}\left[f(x_0, y_0) + f\left(x_1, y_1^{(n)}\right)\right], n = 0,1,2, \dots \quad (8)$$

where $y_1^{(n)}$ is the nth approximation to y_1. The iteration formula (8.14) can be started by choosing $y_1^{(0)}$ from Euler's formula:

$y_1^{(0)} = y_0 + hf(x_0, y_0)$

Example 3:

Determine the value of y when $x = 0.1$ given that $y(0) = 1$ and $y' = x^2 + y$

We take $h = 0.05$. With $x_0 = 0$ and $y_0 = 1.0$, we have $f(x_0, y_0) = 1.0$. Hence Euler's formula gives $y_1^{(0)} = 1 + 0.05(1) = 1.05$

Further, $x_1 = 0.05$ and $f\left(x_1, y_1^{(0)}\right) = 1.0525$. The average of $f(x_0, y_0)$ and $f\left(x_1, y_1^{(0)}\right)$ is 1.0262 . The value of $y_1^{(1)}$ can therefore be computed by using Equation (8) and we obtain

$y_1^{(1)} = 1.0513$

Repeating the procedure, we obtain $y_1^{(2)} = 1.0513$. Hence we take $y_1 = 1.0513$, which is correct to four decimal places.

Next, with $x_1 = 0.05, y_1 = 1.0513$ and $h = 0.05$, we continue the procedure to obtain y_2, i.e., the value of y when $x = 0.1$. The results are

$y_2^{(0)} = 1.1040, y_2^{(1)} = 1.1055, y_2^{(2)} = 1.1055$

Hence we conclude that the value of y when $x = 0.1$ is 1.1055 .

4.5 Runge-Kutta Methods:

As already mentioned, Euler's method is less efficient in practical problems since it requires h to be small for obtaining reasonable accuracy. The

Runge-Kutta methods are designed to give greater accuracy and they possess the advantage of requiring only the function values at some selected points on the subinterval.

If we substitute $y_1 = y_0 + hf(x_0, y_0)$ on the right side of Eq. (7) of 4.4.2, we obtain

$$y_1 = y_0 + \frac{h}{2}[f_0 + f(x_0 + h, y_0 + hf_0)]$$

where $f_0 = f(x_0, y_0)$. If we now set

$k_1 = hf_0$ and $k_2 = hf(x_0 + h, y_0 + k_1)$

then the above equation becomes

$$y_1 = y_0 + \frac{1}{2}(k_1 + k_2) \quad \ldots\ldots\ldots..(1)$$

which is the second-order Runge-Kutta formula. The error in this formula can be shown to be of order h^3 by expanding both sides by Taylor's series. Thus, the left side gives

$$y_0 + hy_0' + \frac{h^2}{2}y_0'' + \frac{h^3}{6}y_0''' + \cdots$$

and on the right side

$$k_2 = hf(x_0 + h, y_0 + hf_0) = h\left[f_0 + h\frac{\partial f}{\partial x_0} + hf_0\frac{\partial f}{\partial y_0} + O(h^2)\right].$$

Since

$$\frac{df(x,y)}{dx} = \frac{\partial f}{\partial x} + f\frac{\partial f}{\partial y}$$

we obtain

$$k_2 = h[f_0 + hf_0' + O(h^2)] = hf_0 + h^2f_0' + O(h^3)$$

so that the right side of Equation (1) gives

$$y_0 + \frac{1}{2}[hf_0 + hf_0 + h^2 f_0' + O(h^3)] = y_0 + hf_0 + \frac{1}{2}h^2 f_0' + O(h^3)$$
$$= y_0 + hy_0' + \frac{h^2}{2}y_0'' + O(h^3)$$

It therefore follows that the Taylor series expansions of both sides of Equation (1) agree up to terms of order h^2, which means that the error in this formula is of order h^3.

More generally, if we set

where $y_1 = y_0 + W_1 k_1 + W_2 k_2$ ....(2a)

$$\left.\begin{aligned} k_1 &= hf_0 \\ k_2 &= hf(x_0 + \alpha_0 h, y_0 + \beta_0 k_1) \end{aligned}\right\} \dots\dots\dots..(2b)$$

then the Taylor series expansions of both sides of the last equation in (2a) gives the identity

$$y_0 + hf_0 + \frac{h^2}{2}\left(\frac{\partial f}{\partial x} + f_0\frac{\partial f}{\partial y}\right) + O(h^3) = y_0 + (W_1 + W_2)hf_0$$
$$+ W_2 h^2\left(\alpha_0\frac{\partial f}{\partial x} + \beta_0 f_0\frac{\partial f}{\partial y}\right) + O(h^3)$$

Equating the coefficients of $f(x, y)$ and its derivatives on both sides, we obtain the relations

$$W_1 + W_2 = 1, W_2\alpha_0 = \frac{1}{2}, W_2\beta_0 = \frac{1}{2}. \dots\dots.(3)$$

Clearly, $\alpha_0 = \beta_0$ and if α_0 is assigned any value arbitrarily, then the remaining parameters can be determined uniquely. If we set, for example, $\alpha_0 = \beta_0 = 1$, then we immediately obtain $W_1 = W_2 = 1/2$, which gives formula equation(1).

It follows, therefore, that there are several second-order Runge-Kutta formulae and that formulae equations (2) and (3) constitute just one of several such formulae.

Higher-order Runge-Kutta formulae exist, of which we mention only the fourth-order formula defined by

$$y_1 = y_0 + W_1 k_1 + W_2 k_2 + W_3 k_3 + W_4 k_4 \dots\dots\dots.(4a)$$

where

$$\left.\begin{aligned} k_1 &= hf(x_0, y_0) \\ k_2 &= hf(x_0 + \alpha_0 h, y_0 + \beta_0 k_1) \\ k_3 &= hf(x_0 + \alpha_1 h, y_0 + \beta_1 k_1 + v_1 k_2) \\ k_4 &= hf(x_0 + \alpha_2 h, y_0 + \beta_2 k_1 + v_2 k_2 + \delta_1 k_3), \end{aligned}\right\} \dots\dots\dots(4b)$$

where the parameters have to be determined by expanding both sides of the first equation of (4a) by Taylor's series and securing agreement of terms up to and including those containing h^4. The choice of the parameters is, again, arbitrary and we have therefore several fourth-order Runge-Kutta formulae. If, for example, we set

$$\left.\begin{array}{llll} \alpha_0 = \beta_0 = \frac{1}{2}, & \alpha_1 = \frac{1}{2}, & \alpha_2 = 1, \\ \beta_1 = \frac{1}{2}(\sqrt{2}-1), & \beta_2 = 0 & \\ v_1 = 1 - \frac{1}{\sqrt{2}}, & v_2 = -\frac{1}{\sqrt{2}}, & \delta_1 = 1 + \frac{1}{\sqrt{2}}, \\ W_1 = W_4 = \frac{1}{6}, & W_2 = \frac{1}{3}\left(1 - \frac{1}{\sqrt{2}}\right), & W_3 = \frac{1}{3}\left(1 + \frac{1}{\sqrt{2}}\right), \end{array}\right\} \ldots\ldots\ldots\ldots\ldots (5)$$

we obtain the method of Gill, whereas the choice

$$\left.\begin{array}{ll} \alpha_0 = \alpha_1 = \frac{1}{2}, & \beta_0 = v_1 = \frac{1}{2} \\ \beta_1 = \beta_2 = v_2 = 0, & \alpha_2 = \delta_1 = 1 \\ W_1 = W_4 = \frac{1}{6}, & W_2 = W_3 = \frac{2}{6} \end{array}\right\} \ldots\ldots\ldots\ldots..(6)$$

leads to the fourth-order Runge-Kutta formula, the most commonly used one in practice:

$$y_1 = y_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \quad \ldots\ldots\ldots (7a)$$

where

$$\left.\begin{array}{l} k_1 = hf(x_0, y_0) \\ k_2 = hf\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1\right) \\ k_3 = hf\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_2\right) \\ k_4 = hf(x_0 + h, y_0 + k_3) \end{array}\right\} \ldots\ldots\ldots\ldots. (7b)$$

in which the error is of order h^5. Complete derivation of the formula is exceedingly complicated, and the interested reader is referred to the book by Levy and Baggot. We illustrate here the use of the fourth-order formula by means of examples.

Example 1:

Given $dy/dx = y - x$ where $y(0) = 2$, find $y(0.1)$ and $y(0.2)$ correct to four decimal places.

(i) Runge-Kutta second-order formula: With $h = 0.1$, we find $k_1 = 0.2$ and $k_2 = 0.21$. Hence

$$y_1 = y(0.1) = 2 + \frac{1}{2}(0.41) = 2.2050$$

To determine $y_2 = y(0.2)$, we note that $x_0 = 0.1$ and $y_0 = 2.2050$. Hence, $k_1 = 0.1(2.105) = 0.2105$ and $k_2 = 0.1(2.4155 - 0.2) = 0.22155$.

It follows that

$$y_2 = 2.2050 + \frac{1}{2}(0.2105 + 0.22155) = 2.4210$$

Proceeding in a similar way, we obtain

$y_3 = y(0.3) = 2.6492$ and $y_4 = y(0.4) = 2.8909$

We next choose $h = 0.2$ and compute $y(0.2)$ and $y(0.4)$ directly. With $h = 0.2$. $x_0 = 0$ and $y_0 = 2$, we obtain $k_1 = 0.4$ and $k_2 = 0.44$ and hence $y(0.2) = 2.4200$. Similarly, we obtain $y(0.4) = 2.8880$.

From the analytical solution $y = x + 1 + e^x$, the exact values of $y(0.2)$ and $y(0.4)$ are respectively 2.4214 and 2.8918 . To study the order of convergence of this method, we tabulate the values as follows:

x	Computed y	Exact y	Difference	Ratio
0.2	$h = 0.1$: 2.4210	2.4214	0.0004	
	$h = 0.2$: 2.4200		0.0014	3.5
0.4	$h = 0.1$: 2.8909	2.8918	0.0009	
	$h = 0.2$: 2.8880		0.0038	4.2

It follows that the method has an h^2-order of convergence.

(ii) Runge-Kutta fourth-order formula: To determine $y(0.1)$, we have $x_0 = 0, y_0 = 2$ and $h = 0.1$. We then obtain

$k_1 = 0.2$
$k_2 = 0.205$
$k_3 = 0.20525$
$k_4 = 0.21053$

Hence

$$y(0.1) = 2 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 2.2052$$

Proceeding similarly, we obtain $y(0.2) = 2.4214$.

Example 2:

Given $dy/dx = 1 + y^2$, where $y = 0$ when $x = 0$, find $y(0.2)$, $y(0.4)$ and $y(0.6)$.

We take $h = 0.2$. With $x_0 = y_0 = 0$, we obtain from (8.21a) and (8.21b),

$k_1 = 0.2$
$k_2 = 0.2(1.01) = 0.202$
$k_3 = 0.2(1 + 0.010201) = 0.20204$
$k_4 = 0.2(1 + 0.040820) = 0.20816$

and

$$y(0.2) = 0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 0.2027$$

which is correct to four decimal places.

To compute $y(0.4)$, we take $x_0 = 0.2, y_0 = 0.2027$ and $h = 0.2$. With these values, Equations. (7a) and (7b) give

$k_1 = 0.2[1 + (0.2027)^2] = 0.2082,$
$k_2 = 0.2[1 + (0.3068)^2] = 0.2188,$
$k_3 = 0.2[1 + (0.3121)^2] = 0.2195,$
$k_4 = 0.2[1 + (0.4222)^2] = 0.2356,$

And $y(0.4) = 0.2027 + 0.2201 = 0.4228$

correct to four decimal places.

Finally, taking $x_0 = 0.4, y_0 = 0.4228$ and $h = 0.2$, and proceeding as above, we obtain $y(0.6) = 0.6841.$

Example 3:

We consider the initial value problem $y' = 3x + y/2$ with the condition $y(0) = 1.$

The following table gives the values of $y(0.2)$ by different methods, the exact value being 1.16722193. It is seen that the fourth-order Runge-Kutta method gives the accurate value for $h = 0.05.$

Method	h	Computed value
Euler	0.2	1.10000000
	0.1	1.13250000
Modified Euler	0.05	1.14956758
	0.2	1.10000000
	0.1	1.15000000
Fourth-order Runge-Kutta	0.2	1.16286242

0.1	1.16722083
0.05	1.16722186

Exercises:

1.Given $\frac{dy}{dx} = 1 + xy,$ y(0)=1, obtain the Taylor series for y(x) and compute y(0,1), correct to four decimal places.

2. Use Picard's method to obtain y(0.1) and y(0.2) of the problem defined by $\frac{dy}{dx} = x + yx^4$, y(0)=3.

3. Using Euler's method, solve the following problems:

(a) $\frac{dy}{dx} = \frac{3}{5}x^3y$, y(0)=1

(b) $\frac{dy}{dx} = 1 + y^2$, y(0)=0

4.Solve, by Euler's modified method, the problem $\frac{dy}{dx} = x + y$, y(0)=0. Choose h=0.2 and compute y(0.2) and y(0.4).

5. Use Runge-Kutta fourth order formula to find y(0.2) and y(0.4) given that $y' = \frac{y^2-x^2}{y^2+x^2}$, y(0)=1.

Unit V

Numerical Solutions of Ordinary Differential Equations: Predictor Corrector method – Milne's Method – Adams-Bash forth method.

Chapter 5: Sections– 5.1 to 5.3

5.1 Predictor-Corrector Methods:

In the methods described so far, to solve a differential equation over a single interval, say from $x = x_n$ to $x = x_{n+1}$, we required information only at the beginning of the interval, i.e. at $x = x_n$. Predictor-corrector methods are the ones which require function values at $x_n, x_{n-1}, x_{n-2}, \ldots$ for the computation of the function value at x_{n+1} A predictor formula is used to predict the value of y at x_{n+1} and then a corrector formula is used to improve the value of y_{n+1}.

In Section 5.2 we describe Milne's method which uses forward differences and in Section 5.3 we derive Predictor-corrector formulae which use backward differences

5.2. Milne's Method:

This method uses Newton's forward difference formula in the form

$$f(x,y) = f_0 + n\Delta f_0 + \frac{n(n-1)}{2}\Delta^2 f_0 + \frac{n(n-1)(n-2)}{6}\Delta^3 f_0 + \cdots \quad \ldots\ldots\ldots..(1)$$

Substituting Equation (1) in the relation $y_4 = y_0 + \int_{x_0}^{x_4} f(x,y)dx$ ……….(2)

we obtain

$$y_4 = y_0 + \int_{x_0}^{x_4}\left[f_0 + n\Delta f_0 + \frac{n(n-1)}{2}\Delta^2 f_0 + \cdots\right]dx$$

$$= y_0 + h\int_0^4\left[f_0 + n\Delta f_0 + \frac{n(n-1)}{2}\Delta^2 f_0 + \cdots\right]dn$$

$$= y_0 + h\left(4f_0 + 8\Delta f_0 + \frac{20}{3}\Delta^2 f_0 + \frac{8}{3}\Delta^3 f_0 + \cdots\right)$$

$$= y_0 + \frac{4h}{3}(2f_1 - f_2 + 2f_3) \quad \ldots\ldots\ldots..(3)$$

after neglecting fourth- and higher-order differences and expressing differences $\Delta f_0, \Delta^2 f_0$ and $\Delta^3 f_0$ in terms of the function values.

This formula can be used to 'predict' the value of y_4 when those of y_0, y_1, y_2 and y_3 are known. To obtain a 'corrector' formula, we substitute Newton's formula from (1) in the relation $y_2 = y_0 + \int_{x_0}^{x_2} f(x,y)dx$ ………….. (4)

and get

$$y_2 = y_0 + h\int_0^2 \left[f_0 + n\Delta f_0 + \frac{n(n-1)}{2}\Delta^2 f_0 + \cdots\right] dn$$

$$= y_0 + h\left(2f_0 + 2\Delta f_0 + \frac{1}{3}\Delta^2 f_0 + \cdots\right)$$

$= y_0 + \frac{h}{3}(f_0 + 4f_1 + f_2)$ ……….. (5)

The value of y_4 obtained from Equation (3) can therefore be checked by using Equation (5).

The general form of Equations. (3) and (5) are:

$$y_{n+1}^{\mathrm{p}} = y_{n-3} + \frac{4h}{3}(2f_{n-2} - f_{n-1} + 2f_n)$$

And $y_{n+1}^{\mathrm{c}} = y_{n-1} + \frac{h}{3}(f_{n-1} + 4f_n + f_{n+1})$

The application of this method is illustrated by the following example.

Example 1:

Solve $y' = 1 + y^2$ with $y(0) = 0$ and we wish to compute $y(0.8)$ and $y(1.0)$.

Solution:

With $h = 0.2$, the values of $y(0.2), y(0.4)$ and $y(0.6)$ are computed and these values are given in the table below:

$k_1 = 0.2,$

$k_2 = 0.2\,(1.01) = 0.202,$

$k_3 = 0.2\,(1 + 0.010201) = 0.20204,$

$k_4 = 0.2\,(1 + 0.040820) = 0.20816,$

$$y(0.2) = 0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 0.2027,$$

x	y	$y' = 1 + y^2$
0	0	1.0
0.2	0.2027	1.0411
0.4	0.4228	1.1787
0.6	0.6841	1.4681

To obtain $y(0.8)$, we use Equation (3) and obtain

$$y(0.8) = 0 + \frac{0.8}{3}[2(1.0411) - 1.1787 + 2(1.4681)] = 1.0239$$

This gives

$y'(0.8) = 2.0480$

To correct this value of $y(0.8)$, we use formula equation (5) and obtain

$$y(0.8) = 0.4228 + \frac{0.2}{3}[1.1787 + 4(1.4681) + 2.0480] = 1.0294$$

Proceeding similarly, we obtain $y(1.0) = 1.5549$. The accuracy in the values of $y(0.8)$ and $y(1.0)$ can, of course, be improved by repeatedly using formula equation (3).

Example 2:

The differential equation $y' = x^2 + y^2 - 2$ satisfies the following data:

x	y
-0.1	1.0900
0	1.0000
0.1	0.8900
0.2	0.7605

Use Milne's method to obtain the value of $y(0.3)$.

We first form the following table:

x	y	$y' = x^2 + y^2 - 2$
-0.1	1.0900	-0.80190
0	1.0	-1.0
0.1	0.8900	-1.19790
0.2	0.7605	-1.38164

Using Equation (3), we obtain

$$y(0.3) = 1.09 + \frac{4(0.1)}{3}[2(-1) - (-1.19790) + 2(-1.38164)] = 0.614616$$

In order to apply Equation (5), we need to compute $y'(0.3)$. We have

$$y'(0.3) = (0.3)^2 + (0.614616)^2 - 2 = -1.532247$$

Now, Equation (5) gives the corrected value of $y(0.3)$:

$$y(0.3) = 0.89 + \frac{0.1}{3}[-1.197900 + 4(-1.38164) + (-1.532247)] = 0.614776$$

5.3. Adams-Moulton Method:

Newton's backward difference interpolation formula can be written as

$$f(x,y) = f_0 + n\nabla f_0 + \frac{n(n+1)}{2}\nabla^2 f_0 + \frac{n(n+1)(n+2)}{6}\nabla^3 f_0 + \cdots \qquad (1)$$

where

$n = \dfrac{x - x_0}{h}$ and $f_0 = f(x_0, y_0)$

If this formula is substituted in $y_1 = y_0 + \int_{x_0}^{x_1} f(x,y)dx$ ……….(2)

we get

$$y_1 = y_0 + \int_{x_0}^{x_1}\left[f_0 + n\nabla f_0 + \frac{n(n+1)}{2}\nabla^2 f_0 + \cdots\right]dx$$

$$= y_0 + h\int_0^1\left[f_0 + n\nabla f_0 + \frac{n(n+1)}{2}\nabla^2 f_0 + \cdots\right]dn$$

$$= y_0 + h\left(1 + \frac{1}{2}\nabla + \frac{5}{12}\nabla^2 + \frac{3}{8}\nabla^3 + \frac{251}{720}\nabla^4 + \cdots\right)f_0$$

It can be seen that the right side of the above relation depends only on $y_0, y_{-1}, y_{-2}, \ldots$, all of which are known. Hence this formula can be used to compute y_1. We therefore write it as

$y_1^p = y_0 + h\left(1 + \frac{1}{2}\nabla + \frac{5}{12}\nabla^2 + \frac{3}{8}\nabla^3 + \frac{251}{720}\nabla^4 + \cdots\right)f_0$ ……….. (3)

This is called Adams-Bashforth formula and is used as a predictor formula (the superscript p indicating that it is a predicted value).

A corrector formula can be derived in a similar manner by using Newton's backward difference formula at f_1 :

$$f(x,y) = f_1 + n\nabla f_1 + \frac{n(n+1)}{2}\nabla^2 f_1 + \frac{n(n+1)(n+2)}{6}\nabla^3 f_1 + \cdots \ldots\ldots (4)$$

Substituting Equation (4) in Equation (3), we obtain

$$y_1 = y_0 + \int_{x_0}^{x_1}\left[f_1 + n\nabla f_1 + \frac{n(n+1)}{2}\nabla^2 f_1 + \cdots\right]dx$$

$$= y_0 + h\int_1^0\left[f_1 + n\nabla f_1 + \frac{n(n+1)}{2}\nabla^2 f_1 + \cdots\right]dn$$

$y_1 = y_0 + h\left(1 - \frac{1}{2}\nabla - \frac{1}{12}\nabla^2 - \frac{1}{24}\nabla^3 - \frac{19}{720}\nabla^4 - \cdots\right) f_1$ ……….(5)

The right side of Equation (5) depends on $y_1, y_0, y_{-1}, \ldots$ where for y_1 we use y_1^p, the predicted value obtained from (3). The new value of y_1 thus obtained from Equation (5) is called the corrected value, and hence we rewrite the formula as

$$y_1^c = y_0 + h\left(1 - \frac{1}{2}\nabla - \frac{1}{12}\nabla^2 - \frac{1}{24}\nabla^3 - \frac{19}{720}\nabla^4 - \cdots\right) f_1^p \quad \ldots\ldots\ldots\ldots(6)$$

This is called Adams-Moulton corrector formula the superscript c indicates that the value obtained is the corrected value and the superscript p on the right indicates that the predicted value of y_1 should be used for computing the value of $f(x_1, y_1)$.

In practice, however, it will be convenient to use formulae (3) and (6) by ignoring the higher-order differences and expressing the lower order differences in terms of function values. Thus, by neglecting the fourth and higher-order differences, formulae (3) and (6) can be written as $y_1^p = y_0 + \frac{h}{24}(55f_0 - 59f_{-1} + 37f_{-2} - 9f_{-3})$ ………… (7)

And $y_1^c = y_0 + \frac{h}{24}\left(9f_1^p + 19f_0 - 5f_{-1} + f_{-2}\right)$ …………. (8)

in which the errors are approximately

$\frac{251}{720}h^5 f_0^{(4)}$ and $-\frac{19}{720}h^5 f_0^{(4)}$ respectively.

The general forms of formulae (7) and (8) are given by

$$y_{n+1}^p = y_n + \frac{h}{24}[55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}]$$

And $y_{n+1}^c = y_n + \frac{h}{24}\left[9f_{n+1}^p + 19f_n - 5f_{n-1} + f_{n-2}\right]$

Such formulae, expressed in ordinate form, are often called explicit predictor corrector formulae.

The values y_{-1}, y_{-2} and y_{-3}, which are required on the right side of Equation (7) are obtained by means of the Taylor's series, or Euler's method, or Runge-Kutta method. Due to this reason, these methods are called starter methods. For practical problems, Runge-Kutta fourth-order formula together with formulae (7) and (8) have been found to be the most successful combination. The following example will illustrate the application of this method.

Example 1:

We consider once again the differential equation given in Example 8.9 with the same condition, and we wish to compute $y(0.8)$.

Solution:

For this example, the starter values are $y(0.6), y(0.4)$ and $y(0.2)$, which are already computed in Example by the fourth-order Runge-Kutta method.

$k_1 = 0.2,$

$k_2 = 0.2\,(1.01) = 0.202,$

$k_3 = 0.2\,(1 + 0.010201) = 0.20204,$

$k_4 = 0.2\,(1 + 0.040820) = 0.20816,$

$$y(0.2) = 0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 0.2027,$$

Using now Equation (7) with $y_0 = 0.6841, y_{-1} = 0.4228$, $y_{-2} = 0.2027$ and $y_{-3} = 0$, we obtain

$$y^{p}(0.8) = 0.6841 + \frac{0.2}{24}\{55[1 + (0.6841)^2] - 59[1 + (0.4228)^2]$$
$$+37[1 + (0.2027)^2] - 9\}$$
$$= 1.0233, \text{ on simplification.}$$

Using this predicted value on the right side of Eq. (8.29), we obtain

$$y^{c}(0.8) = 0.6841 + \frac{0.2}{24}\{9[1 + (0.0233)^2] + 19[1 + (0.6841)^2]$$
$$-5[1 + (0.4228)^2] + [1 + (0.2027)^2]\}$$

$= 1.0296$, which is correct to four decimal places

The importance of the method lies in the fact that when once y_1^{p} is computed from formula (7), formula (8) can be used iteratively to obtain the value of y_1 to the accuracy required.

Exercises:

1.State Adam's predictor – corrector formulae for the solution of the equation

$y' = f(x, y), y(x_0) = y_0$. Given the problem $y' + y = 0, y(0) = 1$.

Find y(0.1), y(0.2) and y(0.3) by Runge-Kutta fourth order formula and hence obtain y(0.4) by Adam's formulae.

2. State Milne's predictor-corrector formulae for the solution of the problem

$y' = f(x, y), y(x_0) = y_0$. Given the initial value problem defined by

$y' = y^2 + xy$, y(0)=1, find, by Taylor's series, the values of y(0.1), y(0.2) and y(0.3).

Use these values to compute y(0.4) by Milne's formulae.

3. Using Milne’s formula, find y(0.8) given that

$\frac{dy}{dx} = x - y^2$, y(0)=0, y(0.2)=0.02, y(0.4)=0.0795 and y(0.6)=0.1762.

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